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Editor

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X- RAY ABSORPTION FINE STRUCTURE STUDIES OF SOME COPPER (II) DITHIOCARBAMATE COMPLEXES

S. Khatri
Professor, Shri RGP Gujarati Professional Institute, Indore
P. A. Kekre
Professor of Physics P. M. B. Gujarati Science College, 01, Nasia Road, Indore

Abstract- X-ray absorption is a powerful technique to explore the environment of the absorbing atom in all type of materials. In present work X-ray absorption find structure studies of some copper (II) dithiocarbamate complexes have been done using seifert X-ray generator and couchois type bent crystal X-ray spectrograph of 0.4m radius. It has been shown that the graphical method proposed by Lytle, Sayer and Stern gives information about the bond length. While the phase parameter of the first co-ordination shell $\propto 1$ and $\beta 1$ Provide of the useful information about the forward and back scattering atoms respectively, the total phase shift $\delta 1$ gives an idea about the periodicity of the X-ray absorption fine structure.

1 INTRODUCTION

In recent year, EXAFS (Extended X-ray Absorption Fine Structure) technique has been developed as a powerful tool for investigation of the geometrical structure of polyatomic, amorphous, and complexes in solid as well as in liquid states1-3. The aim of the present study is to measure the X-ray K-absorption spectra of three copper (II) complexes which are of medicinal interest, namely copper (II) Pepperdine dithiocarbamate)2 [Cu (Pipdtc)2], copper (II) (Hexamethyleneimine dithiocarbomate)2 [Cu (Hmidtc)2] and Cu (II) (N-methylpiperazine dithiocarbamate)2 [Cu(CH3-Pzdtc)2]. Such studies provide useful information on the fine structure of the K-absorption of these Cu (II) complexes. We have derived the phase parameters $\propto 1$ and $\beta 1$ corresponding to the first coordination shell in the present investigation.

2. EXPERIMENTAL DETAILS

A seifert sealed x-ray tube with a tungsten target operating at 16 kV, 60mA was used as the source of continuous radiations A 0.4m couchois type bend crystal transmission spectrograph in its improved form has been used to record the spectra of complexes 4,5.

3. RESULTS AND DISCUSSION

The profiles of the K-absorption discontinuity of the three copper (II) complexes, viz, Cu (Pipdtc) 2, Cu ($Hmidtc$) 2 and Cu ($CH3-pzdtc$) 2 obtained from a number of micro photo meter traces, are shown in Fig. 1.

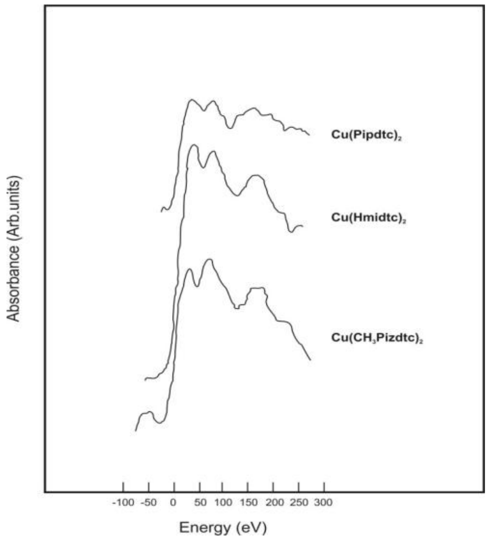

Figure 1

The EXAFS of copper complexes are interpreted in terms of graphical method proposed by Lytle et al6 the values of wave vector k (A0-1) were obtained from the equations.

$$k = (0.263E)^{1/2} \text{ -----------(1)}$$

Where E is the energy (e V) of the peaks in the EXAFS measured from the edge, the k values thus obtained are given in Table 1.

Table 1 Values of wave vector k (A0-1) for major peaks in EXAFS Spectra for the copper K- discontinuity in copper (II) complexes.

n	$k(A^{0-1})$		
	$Cu(pipdtc)_2$.	$Cu(Hmidtc)_2]$	$Cu(CH_3-pzdtc)_2$.
0	2.34	2.42	2.55
1	3.33	3.37	3.33
2	3.97	4.11	4.14
3	4.95	5.22	5.22
4	5.26	6.14	6.28
5	6.30	7.00	7.08
6	6.67	7.21	7.59

The n versus k plots for copper complexes are shown in Fig. 2(a), 2(b) and 2(c)

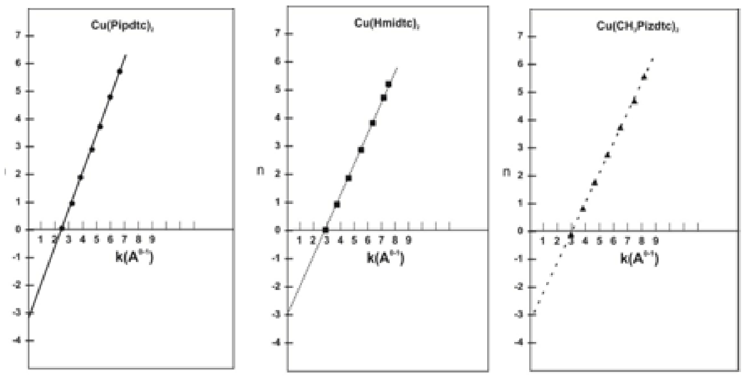

Figure 2(a) Figure 2 (b) Figure 2 (c)

Figure 2(a), Figure 2(b), Figure 2(c) Plot of wave vector k (A0-1) versus principle maxima and minima (n)

Using Fig. 2(a), 2(b), 2(c), and the expression

$$\left(\frac{1}{2}+n\right)\pi = 2k(R_1-\alpha_1)+\beta_1-\pi ------(2)$$

One can easily calculate the phase parameter and the average metal-ligand bond length [7], 10. The factor n gives the position of EXAFS maxima and minima. The results are presented in table 2. More weight age must be given for points with large k values, and if needed some points which occur at small k values may even be ignored since they do not belong to EXAFS region11.

Finally the total phase shift (δ_1) were calculated from the expression[7, 12]

$$\delta_1 = -\alpha_1 k + \beta_1 - \left(\frac{1}{2}\right)\pi ---------- (3)$$

The values of $\delta 1$are listed in table. 3

Table 2 Average values of metal –ligand bond Length (in A0) and phase parameters for cupper (II) complexes

Complex.	$R_{ML}\ (A^0)$	$\alpha_1\ (A^0)$	$-\beta_1$
$Cu(pipdtc)_2$	2.56	0.43	3.2
$Cu(Hmidtc)_2$	2.36	0.43	2.8
$Cu(CH_3 - pzdtc)_2.$	2.40	0.43	2.9

$Rb_{ML}\ (A^o)$Modified Lytle'etal[6] method

$\alpha_1\ (A^0)$ taken from Refs[13-16]

Number of attempts has been made to determine the phase shift theoretically[7, 11, and 12]

According to Teo and Lee[11], the total phase shift experienced by the ejected photoelectron is given by

$$\emptyset_{ab} = \emptyset_a(k) + \emptyset_b(k) - \pi \ldots\ldots\ldots\ldots\ldots\ldots 4$$

Where $\emptyset b$ is the phase of the back scattering amplitude from the neighbour's $\emptyset a$ is the phase shift due to the central atom.

The values of $\delta 1$when plotted against, the wave vector k (Fig.3) gives a curve similar in character to the theoretical curves obtained by teo and Lee11

Table 3 Total phase shift (-$\delta 1$) for copper (II) complexes

N	$-\delta_1$		
	$Cu(pipdtc)_2.$	$Cu(Hmidtc)_2$	$Cu(CH_3 - pzdtc)_2$
0	5.77	5.41	5.56
1	6.20	5.81	5.90
2	6.48	6.14	6.25
3	6.90	6.61	6.71
4	7.03	7.01	7.17
5	7.48	7.38	7.51
6	7.64	7.47	7.73

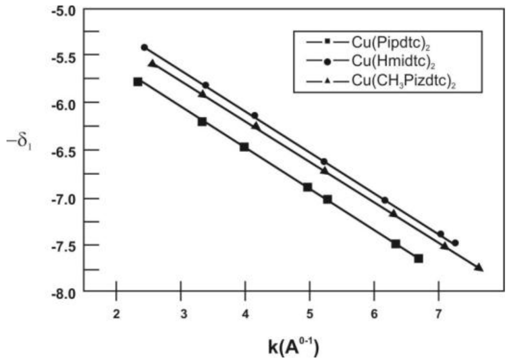

Figure 3 Variation of total phase shift (-δ1), with wave vector (A0−1)

ne may expect that the total phase shift for all the complexes belonging to a given system should be the same. However, this is not the case we find in Fig.3 that δ1versus k plots are different for different complexes. This may attributed to the changes in ligand.

4. CONCLUSION

In the Present work. It has been observed that the graphical method of Lytle et al.

When applied correctly and carefully can give useful information7, 9 about bond length and total phase shift. This method is simple and straight forward and provides a physical picture of the X-ray absorption process in studying systems such as amorphous materials etc.

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XANES ANALYSIS OF CU (II) COMPLEXES

S Mishra[1], A. Mishra[2], Reena Bhatt
[1]Department of physics, Shri Vaishnav Vidyapeeth Vishwavidyalaya, Indore 45331(India)

Abstract- The X-ray absorption spectroscopy is a very strong informative experimental approach to study the coordination geometry and bonding relation in metal compounds. The near edge feature involves the transition from some core state to allowed lowest unoccupied empty states in the valance region of a given atomic center. XANES reveal to identify the allowed transitions and also the mixing or splitting of the final state orbital. [1, 2] Using known structural data, informative deductions on structure-bonding relations have been made. For Cu-containing complexes, Cu K-edge XANES has been widely used to derive information on the electronic and geometrical structure, and some attempts has succeeded in interpreting the absorption features of Cu K-edge XANES spectra. In the present study, it has been reported that Cu K-edge XANES analysis are useful for the quantitative estimation of Cu (II) coordination states in copper metal complexes.

Table1 Copper complexes series, thiosemicarbazide as one of the ligands

S. No.	NAME	ABBREVIATION
1	1-(2,5-dimethoxy-2-nitrobenzylidene) thiosemicarbazide	2,5-dimethoxy
2	1-(3,5-dimethoxy-2-nitrobenzylidene) thiosemicarbazide	3,5- dimethoxy
3	1-(4,5-dimethoxy-2- nitrobenzylidene) thiosemicarbazide	4,5- dimethoxy
4	1-((2-chloroquinolin-3-methylene) thiosemicarbazide	2-chloroquinolin
5	1-((2-chloro-8-methylquinolin-3-methylene) thiosemicarbazide	3-methylene
6	1-((2-chloro-8-methylquinolin-4-methylene) thiosemicarbazide	4- methylene

1 EXPERIMENTAL

(i) Preparation of the sample

The preparations of the complexes were done by chemical root method.

(ii) X-ray spectroscopic studies

The K-absorption spectra were recorded on the synchrotron radiation, i.e., on beam line BL-8 at RRCAT

2 RESULTS AND DISCUSSION

The profiles of the K-absorption discontinuity of five copper complexes are shown in Figure 1.1(a, b, c, d, e).

3 X-RAY K-ABSORPTION PARAMETERS

3.1 Chemical Shift

When an atom irradiated by an energetic beam of particles or photons, an electron from an inner shell can be expelled. When an electron from an outer electronic shell fills the vacancy, it is called characteristic X-ray radiation can be emitted. The energy of the radiation depends on the energy levels of the atom. If continuous X-rays irradiate an atom, then the radiation can absorbed. If the radiation can be absorbed, the energy of the incoming photon is sufficient to ionize the atom or to excite the inner electron to an unoccupied level. This gives rise to an absorption edge in the spectrum for each inner level. The position of the absorption edge gives information about the electron binding energy, i.e., the energy needed to remove the electron from the atom. For several decades, X-ray spectroscopy was the main source of information regarding the atomic structure.

Chemical shift of X.-ray K-absorption edges of complexes and compounds, which are shift of high energy of K-edge, are affected by two factors.

1. The tighter binding of the core level because of the change of the effective charge (or screening) of the nucleolus caused by the participation of the valance electron in the chemical bond formation and
2. The appearance of the energy gap going from metal to compound, which is related to phenomenon such as covalence, effective

charge, coordination number, crystal structure etc. When bonding takes place, the shift in the X-ray absorption edge energy provides valuable information [14, 15] on changes that occurs in the conduction band.

The shift due to chemical combination is on the high-energy side following Agrawal and Verma's rule. [16, 17]. The chemical shift [18-22] and XAS studies [23, 24] have been utilized to obtain important chemical information regarding the coordination in the complexes belonging to transitional metals. The edge shift ΔE_K (known as chemical shift) is defined as follows

$$\Delta E = E_{K(compound)} - E_{K(metal)}$$

The position of the X-ray K absorption edge depends on the valence of the absorbing ion [25]. But valence state is not the only factor that governs the magnitude of the chemical shift. At least four factors that must be considered to explain the chemical shift values in metal complexes as valence state, the effective charge on the central metal ion [26,27], Stereochemistry and ionic bonding.

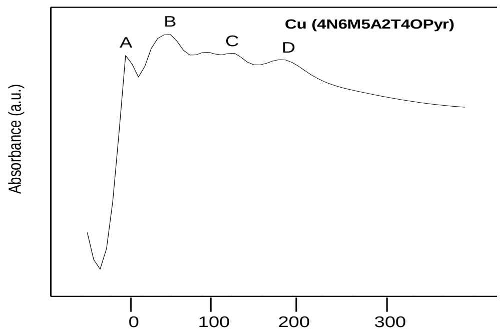

Figure 4.1 c

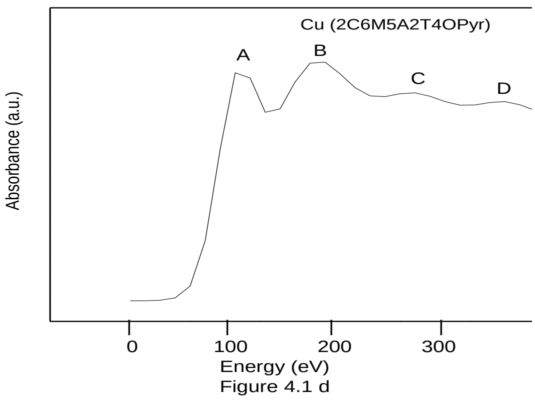

Figure 4.1 d

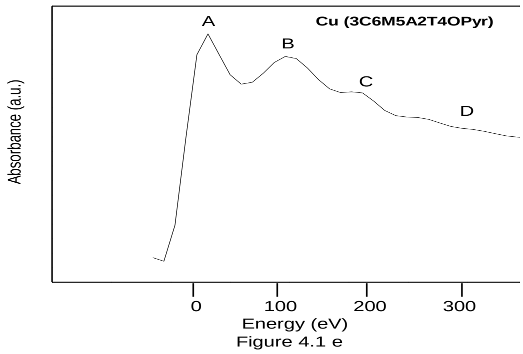

Figure 3.1 (a, b, c, d, e) The profile of the K-absorption discontinuity of five copper (II) Complexes

Table 3.1 X-ray absorption near edge parameters copper (II) complexes.

Name of the Complex	Edge Position E_K (eV)	Chemical Shift $\Delta E_K \sim (\pm 0.2)$	Shift principal absorption Maximum (eV)	Edge Width (eV)
2,5di	8987.5	7.5	27	19.5
3,5di	8991.4	11.4	38	27
4,5di	8988	8	30	22
2chloro	8985.6	5.5	24	19
3chloro	8987	7	29	32
4chloro	8986	6	31	15

Energy of copper absorption edge (EK) present study= 8980 eV [30]

0 100 200 300

Energy (eV)

3.2 Shift of Principal absorption maximum

The shift of the principal absorption maximum depends upon the type of overlap between metal and the ligand orbital's. Greater the overlap of metal d orbital's, the more stable are bonding molecular orbital's. Since transition of principal absorption maximum occurs from 1s to the unoccupied orbitals $(1s \rightarrow T_{1u^*})$ in octahedral complexes the principal absorption maximum shifts to the higher energy. Our value of shift of A in Table 4.1 in case of copper complexes they are ranging from 24 to 38 eV.

3.3 Edge Width

The edge width of the K-absorption edges increase with the increase in covalent character of the bonds provided other factors like molecular geometry etc remain the same. The experimental data of edge-widths of copper complexes are given in Table 4.1. These values are indicating the ionic in nature, looking the values of edge width of the complexes, it is observed that the complex. 3, 5 dimethoxy is more ionic compared to others. This order of the edge width does not match with the order of chemical shift. This is because the edge width does not slowly depend on those factors that are responsible for chemical shift. The values of edge width reported here for copper complexes, indicative of the octahedral structure. This can also be confirmed when there is no splitting of the main edge in the complexes.

4. CONCLUSION

X-ray K-absorption near edge studies of five copper complexes suggests that the chemical shifts values are on the higher energy side. The values reported for copper complexes confirm that these complexes are ionic in nature. The edge width values are found to be on the high energy side. There is no splitting on the main edges of the complexes. These factors suggest the geometrical structure of the complexes to be octahedral. The other important result obtained is that the effective charge is correlated with percentage covalency and chemical shift.

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BIOPHYSICS AND DENTISTRY

Dr. N. G. Toshniwal[1], Dr. Ravindra Manerikar[2], Dr. Shubhangi Mani[3], Dr. Pranit Rathi[4], Dr. Ranjit Kamble[5], Dr. Sunita Shrivastava[6]
Orthodontist, Rural Dental College, Loni

1 INTRODUCTION

For many years there has been an interest in the development of new technologies for use in the oral environment. The focus for a number of methods has been directed toward research, although with the ultimate goal is often applicability to the clinical situation. The paradigm shift in dental caries management from restoration to prevention has led to interest in the ability to detect carious change in the tooth at early stage. In addition it is important to be able to monitor the caries process together with the effect of any strategies aimed at preventing the progression of caries in the clinical situation. Diagnosis therefore not only involves the ability to detect the presence of caries but also to attempt to determine the activity of the lesions that are present. It is against this background that novel applications are existing and also newer biophysical technologies have emerged as aids for diagnosis of dental diseases.

In particular there has been a demand for techniques that allow caries, periodontal diseases, erosion, tooth wear, plaque and calculus to be quantitatively assessed. The development of appropriate techniques offers the research community the opportunity to elucidate in detail not only the disease processes but also the efficacy of agents and therapies to prevent or halt the progression of dental disease. This chapter will outline some of the most useful and most popular current biophysical techniques and evaluate their application for dental research

2 QUANTITATIVE LIGHT-INDUCED FLUORESCENCE AND DENTISTRY

Quantitative light-induced fluorescence (QLD) is an optical technique which uses the natural fluorescence of teeth to differentiate between caries and sound enamel based upon the fact that the fluorescence radiance of a carious spot observed with quantitative light-induced fluorescence is lower than that of surrounding sound enamel.

The dark appearance of a caries lesion observed by quantitative light-induced fluorescence is based on the principle that a demineralized enamel surface restrict the infiltration of light, bring about more scattering of photons entering the carious surface, with the consequent limitation to the chance of a photon being absorbed and fluorescence being transmitted from the demineralized surface than from the surrounding sound surface. Hence the lesion is observed as a dark spot surrounded by highly luminescent sound enamel, the blue and yellow filter combination in quantitative light-induced fluorescence is optimized in such a way that the fluorescence image is completely free of reflections, thereby making caries detection simple and speedier.

The quantitative light-induced fluorescence equipment is made up of a light box accommodate a xenon bulb and a hand-piece, close to in appearance to an intraoral camera, see (Fig. 1).

Light is travelled to the hand-piece via a liquid light guide and the hand-piece carries the band pass filter. Live images are displayed via a computer and accompanying software entitle patient's details to be invaded and individual images of the teeth of curiosity to be captured and stored. Quantitative light-induced fluorescence can image all tooth surfaces not including interproximally. See Fig. 14) for an example of quantitative light-induced fluorescence images that have been joined to produce a assortment on the anterior teeth demonstrating resolution of buccal caries over a 1 month period following supervised brushing. Once an image of a tooth has been captured, the next stage is to analyse any lesions and build a quantitative assessment of the demineralisation condition of the tooth.

Figure 1 QLF Equipment.(a) The QLF unit light box, demonstrating the hand-piece and liquid light guide; (b) A close-up of the intra-oral camera featuring a disposable mirrror tip that also acts as an ambient light shield

These are undertaken using proprietary software and include using a patch to define areas of sound enamel around the lesion of engrossment. Supporting the software uses the pixel values of the sound enamel to re-establish the surface of the tooth and then deduct those pixels which are considered to be lesion. This is managed by a threshold of fluorescence loss, and is generally set to 5%. This means that all pixels with a loss of fluorescence greater than 5% of the average sound value will be considered to be part of the lesion. Once the pixels have been allocate "sound" or "lesion" the software then calculates the average fluorescence loss in the lesion, called as %DF, and then the total area of the lesion in mm2, A the amplification of these two variables results in a third metric output, DQ. When examining lesions longitudinally, the quantitative light-induced fluorescence device employs a video repositioning system that enables the absolute geometry of the original image to be duplicated on subsequent visits. Quantitative light-induced fluorescence has been engaged to observe a range of lesion types. For occlusal caries sensitivity has been reported at 0.68 and specificity at 0.70, and this correlates well with other systems. Correlations of up to 0.82 have also been proclaimed for quantitative light-induced fluorescence metrics and lesion depth. Smooth surfaces, secondary caries and demineralisation adjacent to orthodontic brackets have all been examined.

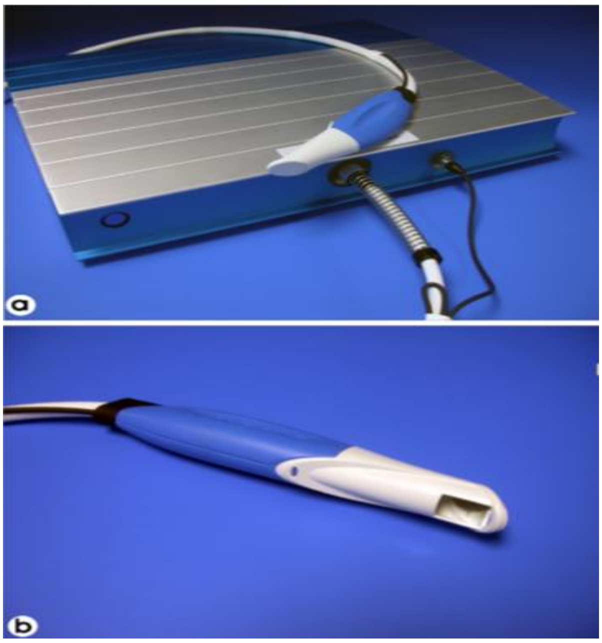

Figure 2 (a) White light image of early buccal caries effecting the maxillary teeth, (b) QLF images taken at the same time as (a), note the improved detection of lesions as a result of the increased contrast between sound and demineralised enamel

The trustworthiness of both stages of the quantitative light-induced fluorescence process; i.e. the image capture and the analysis; have been examined and has been shown to be meaningful. Intra-class correlation coefficients have been proclaimed as 0.96 for image capture, with analysis at 0.93 for intra-examiner and 0.92 for inter-examiner correlations. The quantitative light-induced fluorescence system offers additional benefits beyond those of very early lesion detection and quantification. The images acquired can be stored and transmitted, may be for referral purposes, and the images re-selves can be used as patient motivators in preventative practice.

For clinical research use, the capability to remotely analyse lesions empowers increased legitimacy in trials; permitting, for example, a recite the analyses to be conducted by a unbiased observer. Quantitative light-induced fluorescence is one of the most promising technologies in the caries detection stable at present, although further research is required to demonstrate its ability to correctly monitor lesion changes over time.

2.1 Advantages

- Early caries detection
- Monitoring patients with high caries risk
- Identifying developmental disorders vs carious lesions
- Evaluation of fissure sealants and restorations
- Evaluation of plaque removal

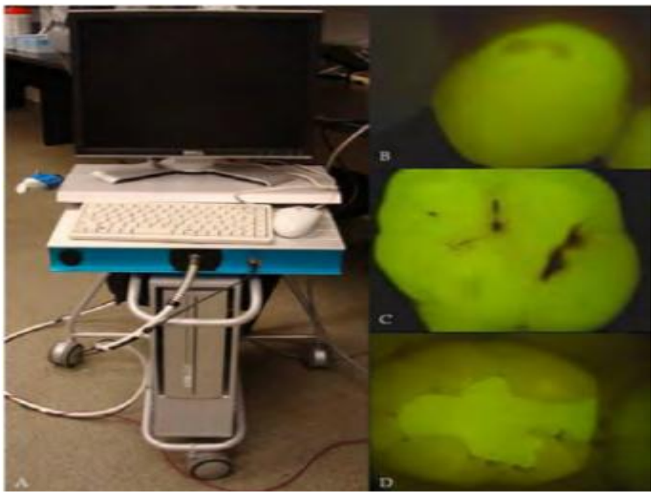

Figure 3 (A) QLF system. (b) Fluorescence image of an enamel caries lesion on the buccal surface (c) Fluorescence image of an occlusal caries lesion. (d) Fluorescence lesion around a composite restoration.

3 DIGITAL IMAGING FIBRE-OPTIC TRANSILLUMINATION

The Footing of visual inspection of caries is beard upon the phenomenon of light scattering. Sound enamel comprises of modified hydroxyapatite crystals that are densely packed, bringing forth a relative transparent structure. The colour of teeth, for example, is strongly motivated by the underlying dentin shade. When enamel is disrupted, for example in the exultance of demineralisation, the penetrating photons of light are scattered (i.e. they change direction, alight do not loose energy) which results in an optical interruption. In normal, visible light, this arrive as a 'whiter' area—the so called white spot.

This appearance is heightens if the lesion is dried; the water is evacuated from the porous lesion. Water has a reciprocal refractive index (RI) to enamel, but when it is evacuated, and reinstate by air, which has a much lower RI than enamel, the lesion is shown more clearly. This demonstrates the importance of assuring the clinical caries examinations are attempted on clean; dry teeth (see Fig. 4).

Figure 1 Fibre-optic transillumination

Fibre optic trans-illumination takes advantage of these optical properties of enamel and strengthens them by using a high intensity white light that is conferred through a small rupture in the form of a dental hand-piece. Light is shone through the tooth and the scattering reaction can be seen as shadows in enamel and dentine, with the device's strength the capability to help in segregation between early enamel and early dentine lesions (see Fig. 5).

A further advancement of fibre-optic trans-illumination is that it can be used for the disclosure of caries on all surfaces; and is especially useful at proximal lesions. The research around fibre-optic trans-illumination is considerably polarised, with a modern review finding a mean sensitivity of only 14 and a specificity of 95 when seeing occlusal dentine lesions, and 4 and 100% for proximal lesions. This is in contradiction to other studies where sensitivity was evidentat 85% and specificity at 99%. Many of the discrepancies can be clarified by the nature of the ordinal scale used to record the subjective visual assortment and the gold standard used to validate the method. However, one would hope fibre-optic trans-illumination to be at least as adequate as a visual examination. Recent developments in ordinal scales for visual assessments, such as the ICDAS scoring system, may enable a more potent framework for visual exams into which fibre-optic trans-illumination can be added (Fig. 5).

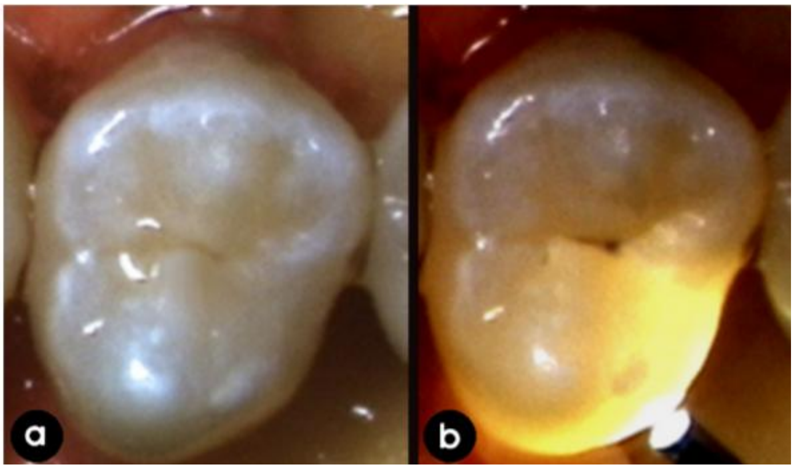

Figure 2 (a) Normal clinical vision, (b) FOTI

One would forecast that fibre-optic trans-illumination would enable discrimination of occlusal lesions to be enhanced (particularly dentine lesions), as well as detection of proximal lesions (in the absence of radiographs) to be greater. As a technique fibreoptic trans-illumination is an obvious choice for adaptation into general practice; the equipment is economical, the learning curve is short and the procedure is not time consuming. Indeed, some work has been undertaken trialling the use of fibre-optic trans-illumination in practice with encouraging results. However with the simplicity of the Fibre-optic trans-illumination system come limitations; the system is subjective rather than objective, there is no continuous data outputted and it is not possible to record what is seen in the form of an image. Longitudinal monitoring is, therefore, a complex matter and some degree of training is required in order to be competent at this level of fibre-optic trans-illumination usage.

In order to address some of these concerns, an imaging version of fibre-optic trans-illumination has been developed; digital imaging fibre-optic trans-illumination. This system comprises of a high intensity light and grey scale camera which can be fitted with one of two heads; one for smooth and one for occlusal surfaces. Images are displayed on a computer monitor and can be archived for retrieval at a repeat visit.

However, there is no attempt within the software to quantify the images, and analysis is still undertaken visually by the examiner who makes a subjective call based on the appearance of scattering. To beaten the anxiety dilemma in fibre-optic trans-illumination, a new method has been tested. Digital imaging fibre-optic trans-illumination is a approach which employs digital image processing for quantitative diagnosis and prognosis in dentistry. It is based on light propagation just below the tooth surface and can be used to regulate lesion depth.

Figure 3 Digital imaging fibre-optic trans-illumination (DIFOTI). (B) Tip for occlusal surfaces

It uses fibre-optic trans-illumination of secure visible light to image the tooth. In this system, light delivered by a fibre-optic is still on the other side of the tooth by a mirror system and documented with a CCD imaging camera, instantaneously. Thus, digital imaging fibre-optic trans-illumination images can be captured in repeatable fashion by maintaining arrangement of a number of imaging control parameters. Then the captured information is sent to a computer for analysis with fateful algorithms, which produce digital images that can be viewed by the dentist and patient in real time or stored for later appraisal.

In addition, this organization can use digital image processing methods to enhance diversity between sound and carious tissues and to quantify condition of incipient, frank and secondary caries lesions on occlusal, adjoining and smooth surfaces. It can also be used to disclose other changes in coronal tooth anatomy, such as tooth fractures and fluorosis. Digital imaging fibre-optic trans-illumination presents higher sensitivity in disclosure early lesions when compared to the radiographic examination and has capability for quantitative monitoring of selected lesions over a period of time.

4 **LASER PROFILOMETRY**

Profilometry measures the amount or mass of a surface. Noncontact optical profilometry grants the non-destructive study of surface things. The measurement of the sample is build on a computer composed traversing stage upon which the sample is systematically browse by either a laser beam using triangulation of the captured image or white light adopting chromatic peculiarity.

The wavelength of the light establish onto the surface measures outpace between the sensor and the sample to detail surface in three-dimensional 3D form. Non-contact profilometry is useful for the laboratory based assessments of depict on small surfaces. Blueprinting has been found to be at the same level as confocal microscopy.

This allocates the depth of the surface to be factored into appraisal of surface change. It has been used in the assessment of erosion, abrasion, abfraction, early dental cavitations, wear of dental restorations, loss of dental enamel during orthodontic treatment as a conclusion of bio film demineralization or enamel bonding techniques, and changes to the form of soft tissues subject to facial prosthetic improvement.

Small samples can be placed in situ for the experimental aspect and then measured in the laboratory. Direct measurement of samples that cannot be removed from the mouth is not achievable. Thus, indirect measurement of, for example, the wear of dental restorations turns necessary. This indirect approach introduces another confounding variable to the efficiency of the technique.

The technique measures flat surfaces more accurately and this leads to in situ samples being ground flat before use. Measurement of a surface that has a natural curve becomes more uncertain. It is a very useful in consolidation with other techniques, particularly when the conditions under examination are compound conditions ourselves. Wear appraisals can be attempted with multiple techniques of which one technique is profilometry.

The combined presentations of erosive demineralization, remineralisation of abraded, eroded enamel, and ultrasonification to study subsurface demineralization of eroded enamel have been effectively studied by using profilometry in combination with assessments of mineral loss or gain. An example is given in combined techniques Fig. 7.

The applications for profilometry in oral research have been demonstrated to commit to any analysis that needs an evaluation of surface topography. The inclusion of an skill to make direct intraoral measurements would be a valuable next step.

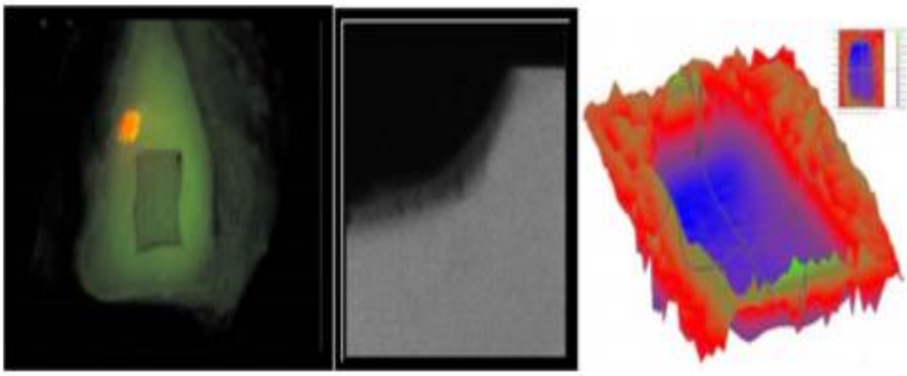

Figure 4 Corrosponding QLF image (left) TMR image (middle) and laser profilometry scan (right) of an bovine tooth

5 TRANSVERSE MICRORADIOGRAPHY

Transverse microradiography (TMR) is a technique that grants the mineral content of the hard tissues to be quantified using x rays. It is based on a approach that has been developed following the work of Angmar and the use of densitometry. The densitometer based systems have been exposed to thorough error analysis. Further important adjustments were made possible following the development of image analysis systems comprising video (CCD) cameras and committed software.

These systems have largely changed the densitometer based systems predominantly due to expanded ease of use. TMR is a lethal technique which requires the samples to be cut into thin sections, polished to give plano parallel sections, adjusted perpendicularly to the anatomical tooth surface. The sections together with a calibration step wedge are brightened by monochromatic x rays, the absorption of which are directly analogous to the optical density of the photographic film or plate and used to calculate mineral content.

TMR is a profitable research tool as a method for directly measuring the mineral content of the dental hard tissues. It is recognized to be a practical and reliable technique convenient for quantifying not only mineral change but also mineral distribution in enamel, dentine, and cementum. As such it has been generally used for in vitro and in situ studies. Unlike profilometry, however, which relies greatly on the need for flat surfaces, TMR is not restricted to non-curved surfaces since a few scans can be made for each microradiograph section Fig. 8.

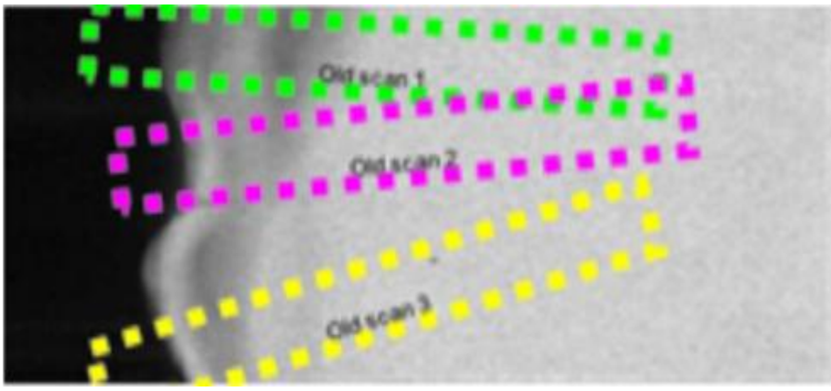

Figure 5 Single TMR scans performed by rotating the image for each scan

Thanks to recent advances in TMR software Fig. 9, curved surfaces can be mathematically flattened to grant accurate mineral content conclusion to be made Figs. 8 and 9.

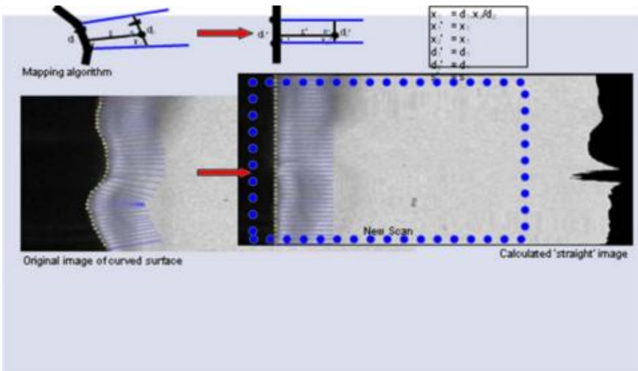

Figure 6 Original TMR analysis of curved surface and using new algorithm

The fact that TMR requires thin sections is clearly a disadvantage in terms of preparation time, destruction of the samples, and the associated limitations with experimental design. Like profilometry, TMR is unable to be used to assess samples that cannot be removed from the mouths of patients or subjects and has to apply experimental designs where lesion parameters can be judged ex vivo. In addition there is a need to analyse control and experimental samples rather than longitudinal analysis of the same tissue.

TMR has become an intensely valuable tool in dental research since it allows very accurate examination of the degree of mineral loss as well as depth and width of lesions.

6 DIAGNODENT

Laser fluorescence device is a non-invasive and quantitative method based on the laser applied fluorescence. The first laser fluorescence device, DIAGNOdent 2095 (KaVo, Biberach, Germany), was advanced in 1998 (Figure 10).

It is based on the assessment of emitted fluorescence from organic components of dental tissues when agitated by a 655nm laser diode (aluminium, gallium, indium and phosphorus - AlGaInP) located on the red range from the visible spectrum. The emitted light grasps the dental tissues through a flexible tip. As the mature enamel is more transparent, this light passes through this tissue without being deflected. In contact with afflicted enamel, this light will be diffracted and dispersed.

The latter is able to excite either the hard dental tissue, concluding in the tissue auto-fluorescence, or fluorophores present in the caries lesions. These fluorophores derived from the products of the bacterial metabolism and has been classified as porphyrins (Hibst et al., 2001). The emitted fluorescence by the porphyrins is gathered by nine concentric fibers and translated into numeric values, which can vary from 0 to 99.

Two optical tips are accessible: tip A for occlusal surfaces, and tip B for smooth surfaces. This device has shown good conclusion in the detection of occlusal caries, however, it might not be used as the only method for treatment decision-making operation (Bader & Shugars, 2006; Rodrigues et al., 2008).

Figure 7 DIGNODENT 2095- A laser fluorescence device for caries detection

This device works on the same principle as the earliest. For this reason, the device was concise and the tips were modified. The tips used in this device are made from sapphire fibre and the same solid single sapphire fibre tip is used for propagation of the excitation and for gathering the fluorescence light, but in opposite leadership and different wavelengths (Lussi & Hellwig, 2006).

There are two tips which can be combined on this device: an occlusal and an approximal tip. However, its achievement in approximal surfaces is still limited. The device weights 140g and only one battery (1,5V) is needed.

Figure 8(A) DIGNODENT 2190 or DIGNODENT pen calibration against the standard ceramic (B) Occlusal tip (c) Approximal tip.

As mentioned before, when a caries lesion or a dental surface is judged by DIAGNOdent, a value between 0 and 99 is observed. This value is, theoretically, associated to the lesion depth. For the values interpretation, several cut-off points have been recommended in the literature, as for DIAGNOdent as for DIAGNOdentpen.

These cut-off points alter from each other in some units in the enamel and dentin. For this reason, is recommended that the clinician acknowledge the values as an interval for the interpretation and also associates clinical and radiographic characteristics for the improve assessment of the lesions. Other factor that potency to be addressed is the presence of stains due to inactive lesions or calculus on the occlusal surfaces due to biological sealing. Both can result in high values of fluorescence and, in consequence, false-positive results.

Therefore, as also approved before visual examination, cleansing of dental surfaces should be performed before laser fluorescence measurements. Besides, after professional prophylaxis using bicarbonate powder or prophylactic paste, it is valuable that the dental surface is rinsed off, so powder or paste does not remain in the fissure or inside micro-cavities. This could agree ait the laser fluorescence measurements (Diniz et al., 2011; Lussi & Reich, 2005).

In conclusion, the clinician who intends to use this method as a auxiliary in the caries detection process should be attentive of the correct device functioning and consider that several factors might hamper the conclusion, such as staining, calculus or powder/paste remnants; calibration policy; and cut-off points variation for enamel and dentin caries.

For this reason, DIAGNOdent or DIAGNOdent pen should not be used as major method for caries disclosure, but as supplementary devices for both visual and radiographic examination. Some situations, in which the professional is in doubt regarding the presence of a caries lesion on a surface free of staining, those devices can be suggested as substitutes for the radiographic examination. .

7 OPTICAL COHERENCE TOMOGRAPHY (OCT)

Optical coherence tomography (OCT) is a non-destructive imaging technique with utilization in medicine for use mainly in ophthalmology, but has operation for imaging other transparent structures as well as semi-transparent structures such as teeth. OCT is able to quantitatively monitor mineral advance in a caries lesion on a longitudinal basis in bovine teeth in vivo. The OCT system used a wavelength of 850 nm but other systems use 1310 nm66 concluding in image depths of 0.6–2.0 mm.

Jones et al. used OCT to successfully examine artificial caries severity and depth in human teeth in vitro. As the application of OCT to dentistry is relatively new, there is still much work to be done to find its full potential. Of clinical relevance is the development of prototype hand pieces for intraoral OCT although no in vivo data have been announced, and as with all optical techniques it is likely that stain will be a confounding factors.

7.1 Electrical caries monitor (ECM)

The relationship between the extent of caries in teeth and electrical support has been investigated. It is possible to estimate caries lesions considering the various parameters affecting the electrical measurements of teeth, such as porosity, surface area of the contact "electrode", the thickness of the enamel and dentin tissues, hydration of the enamel, temperature, ionic gratified the dental tissue fluids, and the maturation time of the tooth in the oral environment (Neuhaus et al., 2009).

The studies on electrical caries monitor device (ECM), (Figure 12) have assessed these parameters in a "site-specific" or "surface specific" mode. This method has shown different results of reproducibility and validity (Huysmans et al., 2005; Kühnisch et al., 2006).

Some in vitro studies indicated that the presence of stain is a confounder for ECM measurements. Besides, the different cut-off hinders for enamel and dentin caries lesions may be useful for stained teeth (Côrtes et al., 2003; Ellwood & Côrtes, 2004). Therefore, its indication in the clinical practice is still unpredictable. Further in vivo studies are necessary in order to make this technology useful in the examinations.

Figure 9 Electrical caries monitor (ECM)

7.2 Ultrasound Techniques

The use of ultrasound in caries detection was first proposed over 30 years ago, although evolution in this field has been slow. The principle backside the technique is that sound waves can pass over gases, liquids and solids and the barrier between them. Images of tissues can be captured by assembling the reflected sound waves.

In order for sound waves to reach the tooth they must pass first through a coupling mechanism, and a number of these have been advised, but those with clinical applications include water and glycerine. A number of studies have been attempted using ultrasound, with differing levels of achievement. One study reported that an ultrasound device could segregate between cavitated and non-cavitated inter-proximal lesions in vitro.

A further study shows that ultrasonic measurements at 70 approximal sites in vitro resulted in a sensitivity of 1.0 and a specificity of 0.92 when compared to a histological gold standard. Further histological acceptance has been attempted by using transverse microradiography and ultrasound. A final in vivo study was attempted using a device described as the Ultrasonic Caries Detector

(UCD) which examined 253 adjacent sites and claimed a diagnostic improvement over bitewing radiography.

7.3 Digital Radiograph

Digital radiography has allow the buried to increase the diagnostic yield of dental radiographs and this has manifested itself in subtraction radiography. A digital radiograph (or a traditional radiograph that has been digitized) is constitute of a number of pixels. Each pixel bears a value between 0 and 255, with 0 being black and 255 being white.

The values in between represent shades of grey, and it can be promptly appreciated that a digital radiograph, with a ability of 256 grey levels has significantly lower resolution than a conventional radiograph that contain millions of grey levels. This would un hold that digital radiographs would have a lower diagnostic yield than that of classical radiographs. Research has confirmed this; with sensitivities and blueprints of digital radiographs being significantly lower than those of regular radiographs when completes small proximal lesions.

However, digital radiographs offer the potential of image enhancement by applying a range of algorithms, some of which appreciate the white end of the grey scale (such as Rayleigh and hyperbolic logarithmic probability) and others the black end (hyperbolic cube root function).

When these enhanced radiographs are estimate their diagnostic performance is at least as good as conventional radiographs, with reported values of 0.95 (sensitivity) and 0.83 (specificity) for a proximal lesions. See (Fig. 13) for an example of this enhancement. When these findings are considered, one must learn that digital radiographs offer a decrease in radiographic dose and thus offer additional assist than diagnostic yield. Digital images can also be accomplish and replicated with abate.

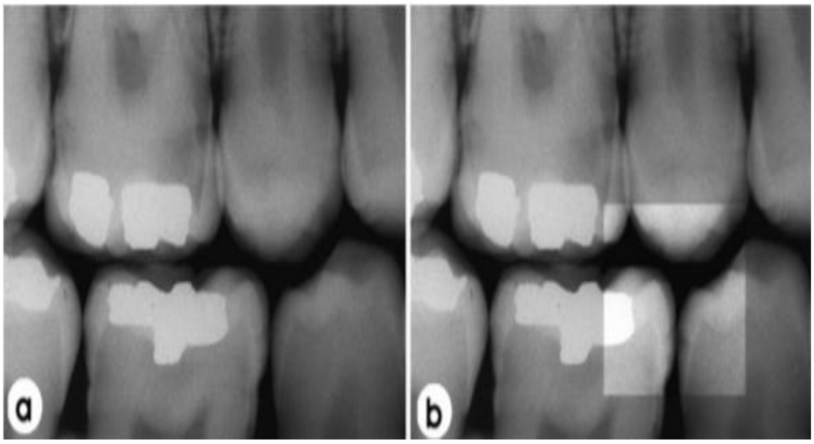

Figure 10 Comparison of regular and enhance digital radiograph. (a) Digital radiograph, (b) Enhance radiograph where the interproximal lesions between first molar and second premolar can be seen more clearly

8 SUBTRACTION RADIOLOGY

A digital radiograph offers a number of conveniences for image enhancement, processing and manipulation. One of the most promising technologies in this regard is that of radiographic subtraction which has been extensively evaluated for both the detection of caries and also the assessment of bone loss in periodontal studies.

The basic premise of subtraction radiology is that two radiographs of the same object can be compared using their pixel values. If the images have been taken using either a geometry stabilising system (i.e. a bitewing holder) or software has been employed to register the images together, then any differences in the pixel values must be due to change in the object.

The value of the pixels from the first object are subtracted from the second image. If there is no change, the resultant pixel will be scored 0; any value that is not 0 must be attributable to either the onset or progression of demineralisation, or regression. Subtraction images therefore emphasise this change and the sensitivity is increased.

It is clear from this description that the radiographs must be perfectly, or as close to perfect as possible, aligned. Any discrepancies in alignment would result in pixels being incorrectly represented as change.

Several studies have demonstrated the power of this system, with impressive results for primary and secondary caries. However, uptake of this system has been low, presumably due to the need for well aligned images. Recent advances in software have enabled two images with moderate alignment to be correctly aligned and then subtracted.

This may facilitate the introduction of this technology into mainstream practice where such alignment algorithms could be built into practice software currently used for displaying digital radiographs. An example of a subtraction radiograph is shown in (Fig.14)

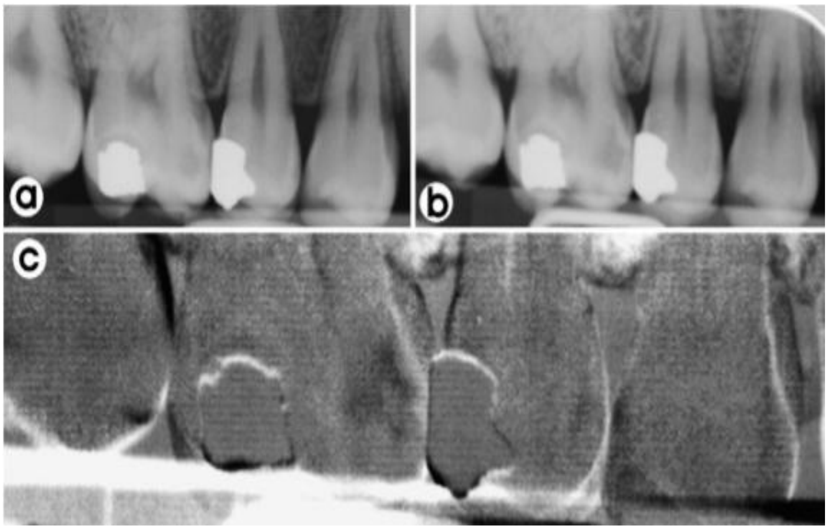

Figure 11 (a) Radiograph showing proximal lesion on mesial surface of first molar, (b) Follow up radiograph taken 12 month later, (c) The areas of different between the films are shown as black i,e in this case the proximal lesion has become more radiolucent

9. CONCLUSION

1. **Quantitative light-induced fluorescence** is one of the most promising technologies in the caries detection stable at present, although further research is required to demonstrate its ability to correctly monitor lesion changes over time.
2. **Digital imaging fibre-optic trans-illumination** presents higher sensitivity in disclosure early lesions when compared to the radiographic examination and has capability for quantitative monitoring of selected lesions over a period of time.

3. The applications for **profilometry** in oral research have been demonstrated to commit to any analysis that needs an evaluation of surface topography.
4. **TMR** has become an intensely valuable tool in dental research since it allows very accurate examination of the degree of mineral loss as well as depth and width of lesion.
5. The clinician who intends to use **DIAGNODENT** as auxiliary in the caries detection process should be attentive of the correct device functioning and consider that several factors might hamper the conclusion, such as staining, calculus or powder /paste remnants; calibration policy; and cut-off points variation for enamel and dentin caries.
6. **Digital radiographs** offer the potential of image enhancement by applying a range of algorithms, some of which appreciate the white end of the grey scale (such as Rayleigh and hyperbolic logarithmic probability) and others the black end (hyperbolic cube root function).
7. **Subtraction radiology** has been extensively evaluated for both the detection of caries and also the assessment of bone loss in periodontal studies.
8. **Optical coherence tomography** (OCT) is able to quantitatively monitor mineral advance in a caries lesion.

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BIOPHYSICS AND TOOTH MOVEMENT- A CRITICAL APPRAISAL

Dr. Ravindra Manerikar
Principal& Professor, Rural Dental College, PIMS, Loni
Dr. N.G. Toshniwal[2]
Professor& HOD, Dept of Orthodontics & Dento-facial Orthopaedics, Rural Dental College, PIMS, Loni
Dr. Shubhangi Mani
Professor, Dept of Orthodontics & Dento-facial Orthopaedics, Rural Dental College, PIMS, Loni
Dr. Vaishnavi Maniyar
PG student, Dept of Orthodontics & Dento-facial Orthopaedics, Rural Dental College, PIMS, Loni
Dr. Sonali Deshmukh
Professor& HOD, Dept of Orthodontics & Dento-facial Orthopaedics, Dr. D. Y. Patil Dental College & Hospital, Pune
Dr. Veera Bhosale
Professor& HOD, Dept of Orthodontics & Dento-facial Orthopaedics, Bharati Vidyapeeth Dental College and Hospital, Pune

1 INTRODUCTION

Biophysics is defined as the stream which studies physics in association with living matter. Therefore, is the study of biologic function, structure, and organization in relation to and by the methods of physics?

Biophysical considerations help in reducing the trial and error method of designing orthodontic appliances. Models of physics and mathematics have been utilized to great advantage to provide needed information for the mechanics of forces and movements required in orthodontics. The concepts in the area of biophysics have been developed by Graber (1961), Bur stone (1962), Haack and Weinstein (1963), and Jarabak and Fizzell (1963). The pattern of forces acting on a tooth is more complex than what is usually comprehended and these acts on the dentition during the entire lifespan. The movement of teeth through alveolar bone is certainly a biological process that occurs when the forces act on the surfaces of the teeth. Forces acting on the teeth can be divided into two categories in a broader sense. One of them includes the natural forces from the oral cavity as a result of normal function, growth and development of the same. Examples of which include force of eruption that acts on each tooth during the stages of its root formation, forces of the tongue, lips and other extra-oral musculature.

Also, during the functions of occluding the teeth and mastication of food, the dentition experiences a variety of forces with varying magnitudes and directions that are intermittently being applied. This also includes the forces of gravity and atmospheric pressure acting on the teeth. The resultant of all these forces is a net horizontal component in the anterior direction which is called as the anterior component of forces. This component is the reason for the forward and mesial movement of the teeth towards the midline.

Apparently, all the forces are in balance since the teeth do occupy positions of seeming equilibrium in the oral cavity. The other category includes the forces from the orthodontic appliances which are applied to correct malocclusions. These appliances deliver forces to the crowns of the teeth when they are in a state of elastic deformation. Though the forces are delivered to the crown, their place of actual action differs and that is the periodontium. This can also be called as the place of reaction to the applied forces by the orthodontic appliances. The magnitude and direction of these forces can be predetermined and controlled rather precisely in many instances, unlike the natural forces. The distribution of orthodontic forces against the alveolar walls of the periodontium determines the pattern of alveolar bone resorption and apposition that makes orthodontic tooth movements possible as a result of applied orthodontic force.

The method of application of forces to the crowns of the teeth is important only when it relates to the pressures and tension area that are created against the wall of each alveolus. The distribution of forces to the alveolar bony walls differs as a result of differing morphology of individual teeth. This depends on the root surface area on which the force is transmitted. Therefore, a constant orthodontic force applied will have varying manifestations depending on the individual teeth. Owing to the general formula, i.e. pressure=force/area, teeth with lesser root surface area or single-rooted teeth will experience greater pressure and vice versa.

The biophysical process consists of the bone resorption and apposition that occurs when a force or force system is applied to a tooth by means of orthodontic appliances. This is a unique aspect of biophysical process related to teeth and periodontium. From a clinical point of view, two aspects of biophysics are of prime concern, First, the type of force system that is required to produce a given centre of tipping, and second, the optimal pressures and stresses in the periodontium that stimulate direct resorption of bone. The first of these aspects is important because it is evident that if the orthodontist could control the location of the centre of tipping, then the desired tooth movements could be achieved more directly, This is true even of bodily movement which is tipping about an axis located at infinity.

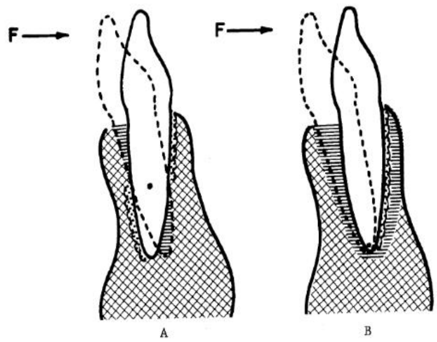
The second consideration is important because, the teeth could move in a more rapid and expeditious manner, with a minimum of damage to the tissues, if the stresses in their respective periodontium were always optimal. The control of the location of the centre of rotation is also of prime concern because to correct mal-positions of teeth, the orthodontist requires a variety of tooth movements such as controlled and uncontrolled tipping, bodily movement or translation, up righting, torquing, intrusion, extrusion, etc. These movements are achieved with a variety of orthodontic forces viz continuous, interrupted or intermittent.

2. HISTORICAL BACKGROUND

To know more about how the forces act and how the bone responds, resulting in tooth movement, let us first review some literature with respect to biomechanics of tooth movement. Then we will see in brief about the appliances that are used for effective tooth movement followed by an example of the same.

Coming to the biomechanics of tooth movement, when it was first discovered that teeth could be moved through alveolar bone, many dentists began to practice what soon became the clinical art of moving teeth in order to correct certain irregularities of the dental arches. Only as a result of the efforts of a few scientific thinkers was orthodontics advanced from purely mechanical considerations to a more professional and scientific endeavour which also placed significance on the biologic principles involved in orthodontic tooth movements.

Biomechanics thus came into being as the science which related mechanics and biologic findings to the correction of malocclusions of teeth. Sandstedt (1904, 1905) was the first investigator to employ a histologic technique to examine orthodontic tooth movement and described the process which is called as “undermining resorption”. With his observations on tipping of the incisors of a dog, he reasoned that in tooth movements, we are dealing with a "double-armed lever", the fulcrum being at about the middle of the root.



Sandstedt (1904, 1905) states that the force, F, produces a tilting around an axis which lies a little apically from the centre of the root. Thus, two regions of pressure and pull arise lying diametrically opposite to each other. In the regions of pressure the old alveolar bone is resorbed (jagged line); in the regions of pull, new bone is added (horizontal shading). The cross-hatching shows alveolar bone without transformation.

Angle (1907), disagreeing with the explanation of tipping given by Sandstedt, carried out another experiment and stated that there is little displacement of the apex because of the greater resistance offered by the thickened bone in that area and by the "innumerable fibers that encapsulate the apex."

Oppenheim (1911) with his studies on a primate (baboon), concluded that the tooth represents a "one-armed lever" with the apex of the root serving as the pivot point or center of rotation. His findings differed sharply from those of Sandstedt.

Oppenheim explained that his preparations showed bone changes almost throughout the entire length of the root, decreasing in intensity from the alveolar border to the root apex. In the area around the root apex, he found that no changes in the bone were observable. Johnson, Appleton and Ritter Shofer (1926) conducted their research of tooth movement on two Macaque Rhesus monkeys using the labio-lingual technique, and their findings were as per those of Sandstedt.

Schwarz (1928) subjected monkeys' teeth to horizontal and oblique forces and analyzed the "tilting" of the tooth that occurred within the alveolus. He found that in tipping a single-rooted tooth, the center of rotation always lays "somewhere in the apical half of the clinical root, and nearer to the middle of the root than the apex."

Kronfeld (1931) confirmed the results of Schwarz's experiment by studying histologic sections of human teeth. Storey and Smith (1952) studied the question of whether there was an optimum force that would cause teeth to move without damage.

Graber (1961) also reported several observations and theories concerning the mechanics involved in tooth movements. He wrote in his textbook that: “A tipping force of moderate-intensity sets up a fulcrum at about one-third the way up the root from the apex. But several factors influence the position of the fulcrum. One is the point of application of force. The closer to the incisal edge the point of force application, the greater the distance of the fulcrum from the apex. The same fulcrum reaction takes place with an increase in the intensity of force application. Heavy forces move the fulcrum away from the apex; light forces move it closer to the apex.”

In comparing tipping to bodily movement, he noted that "clinically, with conventional fixed appliances, a greater force is usually required for bodily movement."

Sicher (1962) described the structure and function of the periodontal ligament. He admits that a one-rooted tooth can be observed to tip around an axis or fulcrum situated somewhere in the middle one-third of the root.

Gantt (1960) had included in his study of tooth movement, a description of the centre of tipping of the mandibular molar teeth during anchorage preparation with light forces. He had noted that the axis of tipping of the anchor tooth occurred more commonly in the apical third of the root than it did in the middle third of the root. His findings were confirmed by similar radiographic studies that followed by Stier (1961), Kemp (1962), Kravica (1963), and Follico (1964). In addition to the studies reporting on the biologic aspects of tooth movement, other investigations were being conducted concurrently to determine the mechanics involved.

A textbook on Dental Orthopedia by Case (1908) included a chapter entitled "Principles of Mechanics in the Movement of Teeth."

From his discussion in this chapter of the different types of tooth movement; of the different kinds of levers; of the relations of power, stress, and movement; of the action line of forces; and of Newton's third law of motion, it is obvious that he was familiar with the true meaning of the word "mechanics" as described by physicists." Fish (1917) summarized the trend of that time when he said: "The influence of technology on orthodontia demands your attention. Engineering methods, applied in the diagnosis and the treatment of malocclusion are producing results that mark the passing of empiricism in orthodontia. Where an art has stood, there is growing up a science." It is significant that in that same year, another article appeared in the International Journal of Orthodontia written by another consulting engineer. Hanau (1917) wrote "Orthodontic Mechanics; Dental Engineering" in which he defined such terms as force, resistance, velocity, work, energy and power, and such concepts as pressure on the root surface, projected root surface area, and volume of absorbed bone tissue."

Stanton (1928), although not an engineer himself, wrote about "Engineering in Orthodontic Diagnosis" and urged the dental and orthodontic societies and all dental schools to employ mechanical engineers to aid in teaching and explaining the engineering principles in dentistry and orthodontics.

Drenker (1956) gave great impetus to the trend toward greater utilization of engineering mechanics in orthodontics. When he began his studies of dentistry and orthodontics, he had already earned two degrees in Mechanical Engineering. He investigated and reported an analytical method for calculating the forces and torques associated with second-order bends.

Weinstein and Haack (1959) stressed the idea that the study of theoretical mechanics, that is, the science of force action, is essential in orthodontics. In addition, they called attention to the need for an understanding of forces relative to the initiation of tooth movement. Particularly they emphasized the importance of the concept of equilibrium which provides a method by which the forces and couples acting in different planes and in different directions can be resolved and better understood. Such forces include not only those acting upon the crowns but also the reaction forces upon the roots.

Teasley, Penley and Morrison (1962) grouped the various means of resolving a force system into three categories: (1) the use of mathematical formulae, (2) physical measurements, or (3) by a combination of the two. They preferred to use physical measurements because it was the most practical method for the evaluation of orthodontic appliances.

In 1963, Weinstein, Haack, Morris, Snyder and Attaway, formulated a hypothesis which they referred to as "an equilibrium theory of tooth position." According to this hypothesis, a tooth is considered to be a "body in the state of rest or equilibrium, when the resultant of all the forces acting on the crown and those developed against the root is equal to zero." If the forces exerted upon the crown have a zero resultant, then the equilibrium of the tooth as a whole does not require the development of reactive forces upon the root. This was validated by a clinical experiment.

Jarabak and Fizzell (1963) placed the greatest emphasis possible on the importance of biomechanics (or biophysics) of tooth movement by devoting four chapters of their textbook to this all-important aspect of orthodontics. They discussed in detail the fundamentals of analytical mechanics, applications of mechanics to orthodontic force systems, elementary strength of materials and biophysical considerations of orthodontic forces. This comprehensive work embodies the most advanced concepts of the nature of orthodontic tooth movements and is, indeed, "a study of the biologic function, structure, and organization (of the teeth and the periodontium) in relation to and by the methods of physics."

Since then a lot of new appliances and techniques have been evolved for carrying out the desired tooth movements for orthodontic treatment but the fundamental basis of all of them will always be covered by the universal laws of physics.

Charles Justin Burstone (1928-2015) has extensively contributed to the field of orthodontics and has helped to develop orthodontic biomechanics on a scientific basis. His research is based on the application of complex mathematical equations and variables combined with laws of physics which are usually known by the engineers and not the orthodontists. He was the first one to research on force-driven or thodontics and the aim of all his research was based on this concept.

Ravindra Nanda (1943-present) has extensive studies on biomechanics to deliver efficient orthodontic treatment. Wide extent of biomechanics has been explained by orthodontists Vijay Jayade and Chetan Jayade as well in a very simplified manner.

3. MECHANCICAL PRNCIPLES IN ORTHODONTICS

Knowledge of the mechanical principles governing forces is necessary for the control of orthodontic treatment. FORCE can therefore be termed as **orthodontic medicine.**

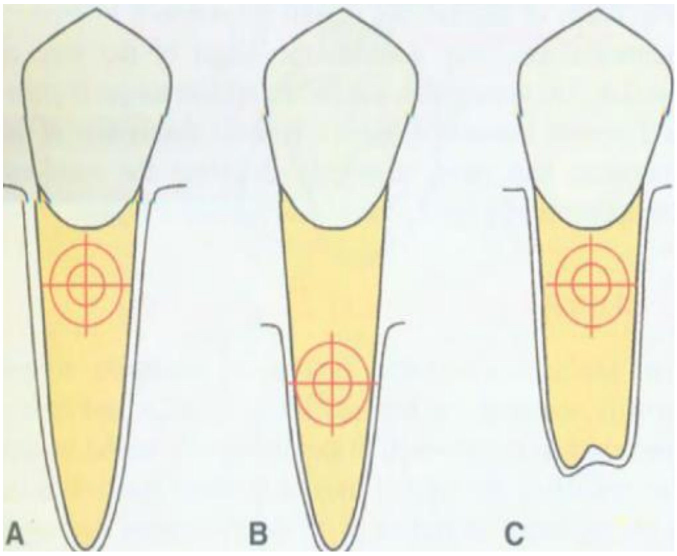
Any movement of teeth in the alveolar bone requires application of force. A complex system of forces is generated within the oral cavity. A clinician needs to analyse these force systems and design them according to the movement of teeth desired. This designing of force systems requires thorough knowledge of mechanics in order to obtain desired tooth movements with negligible side effects. Therefore biophysics is important to understand the application of force, its effect on the teeth and to design force systems which will negate the side effects and provide with necessary desired effects.

Hence we can say that the basis of orthodontic treatment lies in the clinical application of bio mechanic concepts. Mechanics is the discipline that describes the effect of forces on bodies whereas biomechanics refers to the science of mechanics in relation to biologic systems.

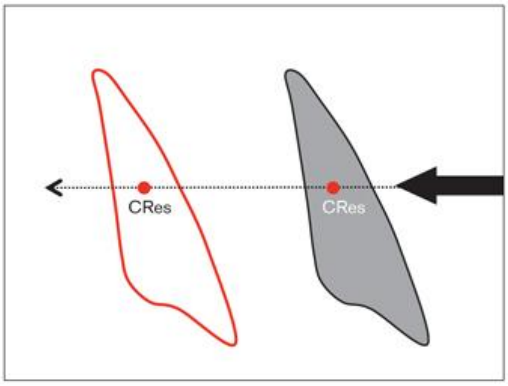
The orthodontic appliances that are selected, inserted, and activated by the clinician produce these forces. The teeth and their associated support structures respond to these forces with a complex biologic reaction that ultimately results in the teeth moving through their supporting bone. This biologic reaction takes place in the periodontium but the cells of the periodontium, which respond to the applied forces, are insensitive to the bracket design, wire shape, or alloy of the orthodontic appliances-their activity is based solelyon the stresses and strains occurring in their environment. Various mechanisms are used to produce these orthodontic force systems. The several ways used to produce these force systems include-the deflection of wires, activation of springs, elastics, etc. which are some of the common methods used for the same. The basic terms of the physics also form the basis of biomechanical principles of orthodontics such as centre of mass, centre of resistance, centre of rotation, line of action of force, vector, resultant vector, moment of force, moment of couple, etc.

Centre of mass is of less importance in orthodontics as a tooth is not a free body. A tooth is encased by the periodontium; therefore using the term centre of resistance becomes more appropriate. A centre of resistance of the tooth is that point on the tooth where a single force applied will produce translation of the tooth i.e. all points on the tooth will move in the same direction and movement that will result will be bodily shift of the tooth without any rotational tendencies.

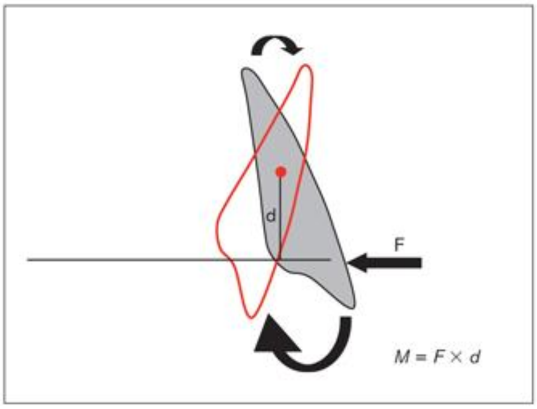
Depending upon the segment of which movement is desired, Centre of resistance can be defined for a single tooth, a group of teeth or the bone in which the teeth are set i.e. if we want to move a single tooth, we will then consider centre of its resistance only to plan the force system. Now to understand further, we will consider movements of a single tooth. As described earlier, orthodontic movements include controlled and uncontrolled tipping, rotation, translation, up righting, torquing, intrusion and extrusion.



Location of centre of resistance varies according to the alveolar bone support. For example, the centre of resistance of a healthy tooth with optimum bone support lays at about 2/5th the length of the root from the alveolar crest to the rooth apex.



In simpler terms, to have bodily movement or translation of a tooth, the line of force has to pass through the centre of resistance of the tooth. Any line of force passing away from the centre of resistance will have a rotational tendency and this moment depends on the distance between the applied force and the centre of resistance. Moment of force is the rotational tendency of the tooth and it is generated when the force is applied at any point that is away from the centre of rotation of the tooth. It can be clockwise or anticlockwise and is calculated by multiplying the force applied and its distance from the centre of resistance.

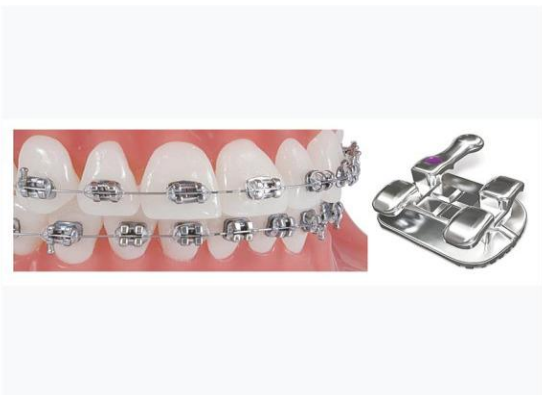


A couple is required to generate pure rotation of teeth around the centre of resistance and it is done by two equal and opposite non-co linear forces. It can also be called as the sum of two moments created by two forces that form the couple. All the force systems work on Newton's third law of motion. Many a times the reaction of forces applied is not desired. In these cases, we obtain anchorage from more rigid structures such as the bone. This method is called as skeletal anchorage. Mini-implants are used in these cases for obtaining such anchorage. These are placed in the bone between the roots of the tooth. Other methods of obtaining absolute anchorage are by using bone screws. Infra-zygomatic bone screws are used in the maxilla and buccal shelf bone screws are used in the mandible.

4. ORTHODONTIC APPLIANCES

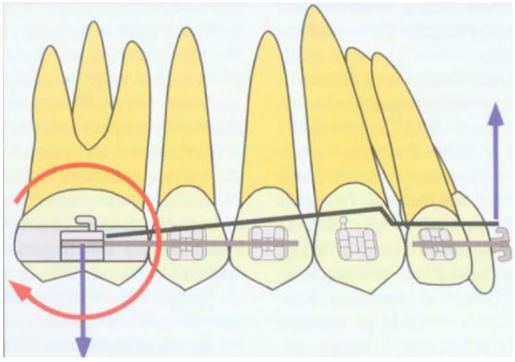
Now coming to the orthodontic appliances that are used to deliver forces, these are the orthodontic brackets which are intricately designed and developed over years as a result of which a sophisticated appliance has come into existence which has also made the work of an orthodontist easier. Fundamentally, the orthodontic bracket acts as a handle, i.e., it is the mechanism through which the clinician attaches wires, springs, elastics, or other devices that exert forces on the teeth. Well, these orthodontic brackets do not work alone, they have to be supplemented by arch wires and other active and passive components which in unison help in delivering the desired forces and creating moments for effective tooth movements.

The orthodontic arch wires are made of different metal alloys such as nickel-titanium, stainless steel, etc according to the nature of use. They also differ in shapes and sizes. The role of the orthodontic wire in treatment is to act as a spring and/or a guide. The force required to deflect the wire into the bracket slot provides the activation energy that will produce the tooth movement. In the elastic range, the strain within the wire is the reciprocal of the strain on the periodontal tooth support. A wide range of factors interact and influence the clinical response. The size and shape of the wire in relation to the bracket slot determines the tooth movement in three dimensions.

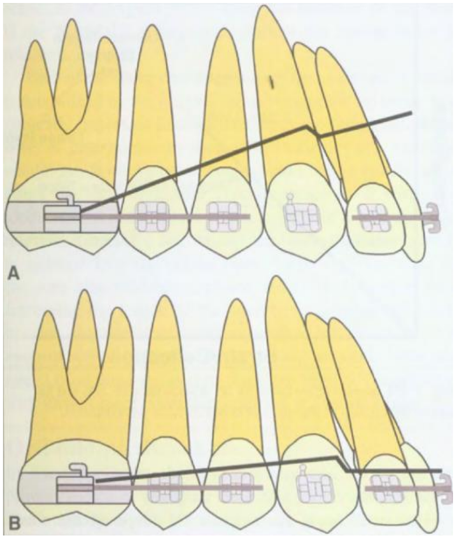


Below is an example of orthodontic tooth movement of maxillary central incisors which were retro lined at the start of orthodontic treatment. The force vectors needed here were that of protrusion (forward movement) and intrusion (upward movement) to get the central incisors into alignment with the other teeth in the dental arch.

The left side pictures are pre-treatment while the right side pictures are those of ongoing treatment. A Rickett's utility arch is used for simultaneous protrusive and intrusive force vectors on the maxillary central incisors. This utility arch works on the bioprogressive therapy principle given by Rickett himself. This utility arch when pasive rests at the desired position of the teeth. Then it is actively engaged into the bracket slots placed on the respective teeth. The elastic deformation produced in the wire tries to resolve itself. And during this attempt it gets the teeth with it to the desired position as predetermined when the wire was passive.



Force systems acting when an intrusion utility arch is in place.



A passive (A) and active (B) intrusion arch

5. CONCLUSION

Force being called as orthodontic medicine has to be judiciously used in appropriate ways in co-relation with the biomechanics described. With forces being applied between optimum pressures that can be handled by the periodontium, produces rapid tooth movement as desired in three dimensions. Force being a physical quantity has to be applied in synchrony with the biologic system to achieve best results.

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