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THEORETICAL STUDY OF PIEZOELECTRIC EFFECTS OF LATTICE VIBRATION IN CARBON NANOMATERIALS

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Abstract: *Carbon Nanotubes has superior properties in reinforce piezoelectric effects to increase mechanical strength at the layer interfaces. The author has proposed the relation between the refractive index of carbon nanotube and piezoelectric lattice vibration coefficient on dispersion relation. We have studied the ionic polarization of carbon materials at optical frequencies which are associated with nano piezo electronics lattice vibration. Recent studies of one of the allotropes of carbon i.e., Graphene have shown the piezoelectric properties. This relation is applied to the study of piezoelectric lattice vibration in carbon nanotubes. This paper presents the Piezoelectric effects on carbon nanomaterial. Using Atomic Force Microscopy, we demonstrated the piezoelectric effect of multi-walled carbon nanomaterial under the compression method. This effect is caused by the incident of light on the surface of materials which leads to coherent acoustic Phonons induced diffraction. This way we evaluate the piezoelectric coefficient in the infrared region on single and multilayer of carbon nanomaterials. This theoretical study offers various fundamental research on advancements in carbon-based nanomaterials piezotronics devices.*

Keywords*, Piezoelectric effect, piezotronics devices, Atomic Force Microscopy, Optical frequency****,*** *Carbon nanomaterials.*

Introduction:

Piezoelectricity is a well-known phenomenon that has recently gained a strong interest in Piezotronics. When piezoelectric material is compressed due to crystal deformation then kinetic energy converts into electrical energy producing electricity this effect is known as the piezoelectric effect. The piezoelectric effect occurs due to the mechanical stress of the materials such stress creates shifting of positive and negative charges on centers of materials resulting in an external electric field, later they detect an external electric field causes lattice deformation in piezoelectric materials this effect is known as Inverse piezoelectric effect [2]. It is derived from the Greek word piezein, which means to squeeze or press, and ēlektron, which means, an ancient source of electric charge [3,4]. Pierre Curie and Jacques French physicists discovered piezoelectricity in 1880[5]. Piezoelectric crystals are electrically neutral. The atoms of these materials are not arranged symmetrically, but their electrical charges are balanced, a positive charge cancels out a negative charge nearby. However, squeezing a piezoelectric crystal deforms the structure, pushing some of the atoms closer together or further apart. The most well-known, first commercially piezoelectric material used in electronic devices is the quartz crystal. Other naturally-occurring piezoelectric materials include tourmaline, topaz, and bones. Researchers have researched the other various crystalline materials, ceramics, semiconductor nanomaterials, polymers, cellulose like Topaz, lead zirconate titanate, quartz, GaAs, InSb, ZnO and GaN, etc. have piezoelectric properties which are applicable in various field.

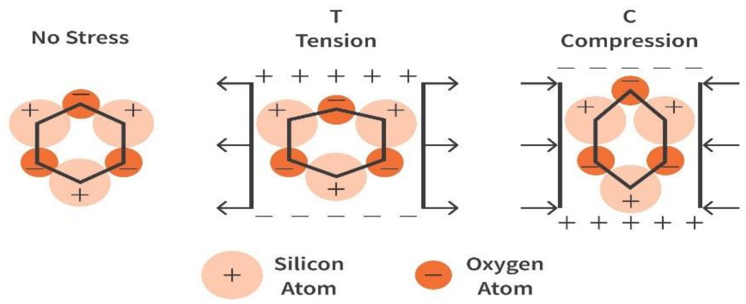

Fig.2 Piezoelectric effect in Quartz [6]

The piezoelectric effect is absent in those materials which have a small surface/volume ratio to electromechanical properties of materials [7]. This area of research is specifically based on the study of the piezoelectric effect on Carbon nanomaterials which leads to a new area of research i.e., nanopiezotronics [8]. To make Carbon as piezoelectric material needs approx. 25 percent strain, higher elasticity, and strength. It has been already theoretically confirmed on one of the allotropes of carbon nanomaterial (Graphene) which shows a piezoelectric effect under compression [9]. In infrared frequency regions, there are two kinds of polarization in dielectrics in response to the electric field of the incident light, electronic and ionic polarization. Ionic polarization causes piezoelectric vibrations in piezoelectric crystals. Propagation of light through piezoelectric materials inevitably induces periodic elasticity and dynamic grating structure of carbon nanomaterials at the frequency of the incident light. This effect is referred to as optical piezoelectricity at the visible frequency at which the ionic polarization responds to the variation of the incident field in the infrared region. At the low frequency, we cannot determine the piezoelectric coefficient thus piezoelectricity of carbon materials can be enhanced in the infrared region [10]. As piezoelectricity is a deformation-induced process, for this we need highly flexible devices nanostructured materials, here we study piezo lattice vibrations in carbon nanomaterials. Recent studies show that each carbon atom of nanomaterial produced its electric moment when its electric field is nearly zero due to its symmetry in the cylindrical form [11]. If there is some deformation in its symmetry then these carbon nanomaterials show the piezoelectric effect on their surface in the presence of an internal electric field [11]. The presence of piezoelectric effect in Carbon nanomaterials has shown other characteristics like hysteresis of voltage and current emission with electric parameters. when we increase the strain/bending of carbon nanomaterials then the piezoelectric coefficient decreases at the surface of materials. The piezoelectric coefficient of carbon nanomaterials is up to 0.107 ± 0.032 C/m2 [12].

Theoretical Approach

Piezoelectricity is the combined effect of Hooke's Law for linear elastic materials and the linear electrical behavior of the material.

$S=sT$

$S_{ij}= \Sigma_{kl}\, s_{ijkl}\, T_{kl}$ (1)

Where S is the linearized strain, s is compliance, T is stress

$D= \mathcal{E}E$

$D_i = \Sigma_j\, \mathcal{E}_{ij}\, E_j$ (2)

where **D** is the electric flux density, **ε** is the permittivity, and **E** is the Electric Field Strength

When equations (1) and (2) are combined they form Strain- charge Equation which is given as

$S_{ij} = \Sigma\, s_{ijkl}\, Tkl + \Sigma\, d_{ijk}\, E_k$

$D_i = \Sigma\, d_{ijk}\, Tjk + \Sigma\, \mathcal{E}_{ij}\, E_j,$

There are four Piezoelectric coefficients, d_{ij}, e_{ij}, $g_{ij,}$ and h_{ij} defined as

$d_{ij} = (\partial Di/\partial Tj)E = (\partial Sj/\partial Ei)T$ (3)

$e_{ij} = (\partial Di/\partial Sj)E = -(\partial Tj/\partial Ei)S$ (4)

$g_{ij} = -(\partial Ei/\partial Tj)D = (\partial Sj/\partial Di)T$ (5)

$h_{ij} = -(\partial Ei/\partial Sj)D = -(\partial Tj/\partial Di)S$ (6)

The first set of four terms is related to the direct piezoelectric effect and the second set of four terms is related to the converse piezoelectric effect. We calculate piezoelectric coefficients d_{ij} from electrostatic lattice constants [13]. We can also determine the piezoelectric strain constant using applied force on the surface of carbon material with the resulting charge, the equation is given below.

$D_{ij} = Q/F$ (7)

The appearance of nanoparticles in carbon phases acting as nucleation allows for the growth of crystallites in smaller crystal sizes and greater uniformity, the more uniform materials possess smaller crystallites which have a great advantage for charge storage capacity [16]. When the d_{ij} piezoelectric coefficient provides charge generated per unit applied to force the efficiency of energy conversion can be measured through the mechanical- electrical coupling factor k can be expressed as

$$K_{ij} = d_{ij}/\sqrt{\varepsilon_0 \varepsilon_r S_{ij}} \qquad (8)$$

Where k_{ij} is the coupling coefficient, ε_r is the relative dielectric constant, S_{ij} is strain strength and ε_0 is the permittivity of free space. This resulting larger mechanical energy and strain, and a good amount of charge is produced while the increase in value of the dielectric constant.

$S_{ij} = 48{,}000 KNm.Kg^{-1}$

$\varepsilon_r = 3960 \pm 450$

$\varepsilon_r = 1$

$\varepsilon_0 = 8.8542 \times 10^{-12}$ F/m

Using these values in equation (8) we can calculate the piezoelectric coefficient of singled and multi-walled carbon nanomaterials.

For single-walled carbon nanomaterials, we took the value of strain strength as 3960, and for multi-walled carbon nanomaterials, strain strength is 4960. At these values, we found the piezoelectric coefficient of carbon materials in singled and multi as 1296.99Pc/N and 1451.55Pc/N.

We can also determine the piezoelectric coefficient of carbon nanomaterial using piezoresponse force microscopy, the piezoelectric coefficient of aligned carbon material is determined with the help of the Current-Voltage technique method

Table.1 coupling coefficient values for single-Walled and Multi-Walled carbon nanomaterials at different weight percentages.

Wt %	0	0.1	0.2	0.3	0.4	0.5
Multi-Walled	30	33	64	60	69	72
Single-Walled	32	44	55	52	58	63

Results and Discussions:

In the analysis of carbon nanomaterials of singled and multiwalled the maximum values of coupling coefficient at wt% of 0.5, SW carbon nanomaterials performance is lower than multi-walled nanomaterials of carbon resulting in a greater retention of low mechanical compliance, and dielectric constant shows bamboo-like defects in the multiwalled structure, they have metallic chirality in layers of carbon materials. The multi-walled structure of carbon shows different defects in form of modes like D and G modes with lengths of 1.4 – 0.2 micrometers and diameters of approx. 44nm [14]. The study shows that when a sample of carbon nanomaterial is examined under atomic force microscopy the piezoelectric effects show on the upper layer of material when applied force increases the piezoelectric effects increase gradually up to 20nA. therefore, a positive charge begins to predominate at the upper surface of the sample which results in a small increment in current and negative charges begin to predominate at the below surface of the material which reduced the piezoelectric charge [15]. The piezoelectric effect depends on the value of Magnitude and bending strength of carbon materials, with the help of calculated values of the piezoelectric coefficient of singles and multiwalled carbon nanomaterials are 1296.99 and 1451.55 thus, the results show that the multiwalled carbon nanomaterials show larger value than singled layer nanomaterials, so multiwalled carbon nanomaterials is much more useful in nanopiezotronic devices.

Conclusions:

The purpose of this paper is to describe the theoretical confirmation of piezoelectric lattice vibration in single-walled and multi-walled carbon nanomaterials. The piezoelectric effect in carbon materials is very useful in various applications in detecting sound. piezoelectric devices electronic frequency generators and ultra-fine focusing and alignment of optical assemblies among others all exploit piezoelectric technology. It is also the basis of several scientific instrumental techniques with atomic resolution, such as scanning and tunnelling microscopes. The fundamental lattice vibrations of carbon material in the infrared frequency range have been intensively investigated by analysis of the infrared region. The research on the piezoelectric properties of carbon nanomaterials can be used to create nanopiezotronic devices like memory devices that exceed storage speed.

References:

[1]. Priyanka Sahare, Bijay Kumar Sahoo, Piezoelectric lattice vibrations in GaN at optical frequencies, (2022)

[2]. Z.L. Wang, Adv. Mater. 19(6) (2007) 889-892.

[3]. Harper, Douglas. "piezoelectric"

[4]. Liddell, Henry George; Scott Robert; A Greek- English Lexicon at the Perseus Project.

[5]. Manbachi, A. & Cobbold, R.S.C. (2011). "Development and Application of Piezoelectric Materials for Ultrasound Generation and Detection". Ultrasound.

[6]. JR Bishop - Tectonophysics, 1981 – Elsevier

[7]. Zhang, J.; Wang, C.; Bowen, C. Piezoelectric effects and electromechanical theories at the nanoscale. Nanoscale **2014**, 6, 13314–13327.

[8]. Wang, Z.L. Nanopiezotronics. Adv. Mater. **2007**, 19, 889–892.

[9]. Wang, X.; Tian, H.; Xie, W.; Shu, Y.; Mi, W.-T.; Ali Mohammad, M.; Xie, Q.-Y.; Yang, Y.; Xu, J.-B.; Ren, T.-L. Observation of a giant two-dimensional band-piezoelectric effect on biaxial-strained graphene. NPG Asia Mater. **2015**, 7, e154.

[10]. B. Donovan, Lattice Vibrations (1971).

[11]. Kvashnin, A.G.; Sorokin, P.B.; Yakobson, B.I. Flexoelectricity in carbon nanostructures: Nanotubes, fullerenes, and nanocones. J. Phys. Chem. Lett. 2015

[12]. Ilina, M.V.; Blinov, Y.F.; Ilin, O.I.; Rudyk, N.N.; Ageev, O.A. Piezoelectric effect in non-uniform strained carbon nanotubes. IOP Conf. Ser. Mater. Sci. Eng. 2017

[13]. Kochervinskii, V. (2003). "Piezoelectricity in Crystallizing Ferroelectric Polymers". Crystallography Reports.

[14]. Ouyang Y., Cong L.M., Chen L., Liu Q.X., Fang Y. Raman study on single-walled carbon nanotubes and multi-walled carbon nanotubes with different laser excitation energies. Phys. E Low-Dimens. Syst. Nanostruct. 2008.

[15]. Gavrilov S.A., Gromov D.G., Koz'min A.M., Nazarkin M.Y., Timoshenkov S.P., Shulyat'ev A.S., Kochurina E.S. Piezoelectric energy nanoharvester based on an array of ZnO whisker nanocrystals and a flat copper electrode. Phys. Solid State. 2013.

[16]. M. Ullah, A. K. Kadashchuk, P. Stadler, A. Kharchenko, A. Pivrikas, C. Simbrunner, N. S. Sariciftci, and H. Sitter, Mater. Res. Soc. Symp. Proc. 1270, 1270–II06 (2010).