



**ORIGINAL ARTICLE**

**A Review of Experimental and Theoretical Studies of Nanomaterials under Variation of Temperatures and Pressures**

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**ABSTRACT**

*Given the significance of nanomaterials and their applications in science and technology, the examination of the temperature and pressure dependency of thermophysical characteristics is of current interest to those working in the domains of nanoscience and technology. Many experimental approaches have been developed to manufacture and analyse nanomaterials, providing experimental data for future theoretical study. As a result, various theoretical techniques for studying the thermophysical characteristics of nanomaterials at high temperature and high pressure have been presented throughout the last decade. Researchers evaluate the literature on experimental and theoretical investigations of nanomaterials under temperature and pressure variations in this publication. And concluded that there is still room to research the thermo-physical characteristics of nanomaterials for which no acceptable model theory could produce satisfying findings when subjected to high temperatures and high pressure. There were some flaws in the earlier scientists' theory-models.*

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**INTRODUCTION**

The many techniques to studying the thermodynamic characteristics of nanomaterials, which had previously been handled individually, are united. Several theoretical and experimental researches on the thermodynamic characteristics of nanomaterials have been conducted during the last two decades. Earlier theoretical models were based on the uncertainty of prospective parameters and involved time-consuming calculation, resulting in not only computational complexity but also inaccuracy in findings.

Recent advancements in theoretical and experimental methodologies have resulted in major changes in our knowledge of the physical and chemical characteristics of materials at high temperatures and pressures. The thermal equation of state, along with the crystal structure, is one of the most essential parameters in high-temperature and high-pressure research. The A material's equation of state specifies the relationships between its thermodynamic variables, namely volume, pressure, and temperature. Thermal equations of state investigations are important because pressure and temperature modify interatomic distances, causing changes in structure, bonding, and electronic configurations Dubrovinsky (2002). The benefits of the equation of state include the ability to forecast extrapolation and interpolation of values when experimental data is missing. Murnaghan (1944) obtained the fundamental equation of state by assuming that bulk modulus is a linear function of temperature at constant pressure. Murnaghan's equation of state proved extremely effective in understanding the thermophysical

characteristics of bulk materials. However, when there was significant compression, the Murnaghan equation of state was unable to adequately characterise the reference isotherm, preventing extrapolation to higher temperatures. Based on only three equilibrium properties at a single reference temperature, the Vinet equation of state was able to predict the high temperature features of the equation of state. It was expected that the thermal pressure is volume independent and linear with temperature above the Debye point. It predicted not only the pressure volume relation at high temperatures, but also the thermal expansion, isothermal bulk modulus, and zero pressure value of the isothermal derivative of the isothermal bulk modulus. Singh and Gupta recently obtained the isobaric integral form of the equation of state in which they assumed the Anderson Gruneisen parameter to be temperature dependent Singh and Gupta (2003).

Many experimental and theoretical researches have been conducted over the years to study the thermodynamic properties of nanomaterials under the impact of high temperature and pressure. Many innovative nanoparticles, however, still need the investigation of temperature and pressure dependent elastic characteristics nanometrials. The thermal and structural stability of nanocrystalline materials is of great interest since it allows us to comprehend intrinsic micro-features, allowing us to develop better systems due to broad applications in practically every aspect of nanotechnology, with expected outcomes

## HISTORY

Rechar Feynman, a physicist, originally proposed the notion of nanoscience and technology in 1959 in his address "there is plenty of room at the bottom," in which he envisioned the direct manipulation of atoms that may be produced. Norio Taniguchi used the word "nanotechnology" for the first time in history in 1974, claiming that scientists have developed the ability to view and manipulate materials at the nanoscale scale. During 1980-81, the Tunneling Electron Microscope (TEM) and Scanning Electron Microscope (SEM) were invented, ushering in a new era of nanotechnology. The discovery of these two optical electron microscopes enabled unforeseen or unexpected imaging of individual atoms or molecules, motivating the inventors to design the bottom-up approach for nanomaterial synthesis. Kroto *et al.* (1985) developed the bucky ball structure known as fullerene in 1985. Fischer *et al.* (1991) Fullerene is made up of 60 carbon atoms that are joined together to form a cage-like structure with 20 hexagons coupled with 12 pentagons by Vander Waals interactions. Fullerene's molecular structure has the symmetry of a soccer ball and is composed of  $sp^2$  like bonding structure. The discovery of fullerene led to the discovery of carbon nanotubes, which have significant technical implications in engineering and medical science. Nanominerals are crucial in understanding the dynamics and development of the earth's lower mantle under high temperature and pressure. The study of minerals under high temperatures and pressures is thus essential for understanding the science of the earth's interior. The physical characteristics of nanomaterials and nanominerals under high temperature, such as thermal conductivity, electrical conductivity, thermal expansion, specific heat, bulk modulus properties, and so on, reveal an intriguing behaviour. It is therefore crucial and required to evaluate the thermal characteristics of nanomaterials in order to employ them in nanodevices to monitor various physical properties at high temperatures without destroying the materials' structure and size.

Foresterite ( $Mg_2SiO_4$ ) and Faylite ( $Fe_2SiO_4$ ) are two minerals that are commonly referred to be olivine. Faylite is rich in iron whereas Foresterite is Mineral high in magnesium. Forest rite may be found in ultra-igneous rocks, marbles, and iron-nickel meteorites. The study of these minerals at high temperatures is critical because temperature and pressure dependent data are highly relevant and vital for examining deep studies in the field of earth science. Mineral rheological characteristics are highly influenced by grain size Frost *et al.* (1982). Though the physical characteristics of earth

minerals (bulk) with size structures ranging from micro to millimetres are thoroughly researched, theoretical research on nanominerals is still required for future discovery.

Nanocrystalline Bhagwat and Ramaswamy (2007) use amorphous citrate to generate zirconia powder with relatively thin particle size. XRD determines the crystalline size, while TEM determines the particle size with a high degree of accuracy. The inter-atomic separation rises with increasing temperature, indicating that zirconia is not as stiff as other nanocrystals. The stiffness of a zirconia nanoparticle, on the other hand, is greater than that of the bulk crystal. Zinc oxide (ZnO) is a semiconducting ionic crystal that exhibits a fast shift in thermal expansion with temperature Petre Sokolov *et al.* (1999). At high pressure, ZnO has a wurtzite structure that converts into rocksalt, but when the pressure is reduced, it reverts to a wurtzite structure. Petre S. Sokolov *et al.* (1999) as well as Seelaaboniya *et al.* (2005), investigated the thermal expansion and elastic behaviour of ZnO-rocksalt at high temperatures. They discovered that in the ZnO-rocksalt phase, the elastic constants and thermal expansion coefficient rise with increasing temperature, but in the Wurtzite phase, the growth is relatively sluggish. Zinc oxide has several uses, including UV lasers, transparent conducting films, and sunscreen coatings.

TiO<sub>2</sub>, a semiconductor with a huge energy band gap of 3.2 eV, is an optical material because of its high refractive index. It appears in polymorphs in the earth's mantle, and the most prevalent natural polymorphs are rutile, anatase, and brookite. Anatase is metastable, whereas rutile is stable. It has potential uses in electronics, most notably in the fixation of nitrogen to make hydrogen gas. The investigation of the thermal characteristics of n-nickel oxide has also piqued the interest of researchers since it has several potential in microelectronic packaging. It possesses beneficial magnetic and optical characteristics, such as the optical Fibers that aid in the investigation of various forms of nanocomposites, such as aluminium composites and nanopolymers utilised in electronic communication. Because of its high stiffness and thermal conductivity, aluminium composites are employed in field emission devices. Under high temperature and pressure, nanometals such as silver (Ag) and gold (Au) exhibit unique optical, electrical, and thermal characteristics. These metals' electrical and thermal conductivities rise with temperature, in contrast to bulk silver and gold metals, albeit their thermal expansion coefficients do not alter considerably when compared to bulk metals. Antimicrobial coatings, wound dressing, medication delivery systems, and biomedical devices are the most typical applications for silver and gold nanoparticles.

Graphene has a negative thermal expansion coefficient with a temperature range of 0-900K (13nm). Mounet *et al.* (2005) used first principles calculations to calculate the thermal expansion coefficient of graphene and projected that graphene has a negative TEC at least up to 2500K. Bao *et al.* (2009) measured the TEC in the temperature range 300-400K by measuring the slight change in the sagging of a graphene piece dangling above a trench and found that it is negative only up to 350K. However, it is unclear whether the disparity between theory and practical evidence stems from inaccuracies in experimental observations or from constraints in theoretical calculations.

## EXPERIMENTAL REVIEWS OF NANOMATERIALS

Anna Mchale and Robert S. Roth (1986) explored the low temperature phase relationship in the ZrO<sub>2</sub> -TiO<sub>2</sub> system experimentally and presented a novel phase diagram for the aforesaid system.

Turi *et al.* (1995) determined the linear thermal expansion coefficient of a porosity-free electroplated nanocrystalline material at temperatures ranging from 40K to 500K. The isobaric specific heat of Ni for nano Ni is claimed to be between 2.5 and 5% higher than for bulk Ni. However, at 350K, the thermal expansion of nanocrystalline- (Ni-Fe) is seen in decreasing order, which can be ascribed to alloying processes.

Maniwa *et al.* (2001) have determined thermal expansion coefficient of single walled nanocarbon tube bundles as  $(-0.15 \pm 0.20) \times 10^{-5}$  (1/K) and  $(0.75 \pm 0.25) \times 10^{-5}$  (1/K) for the triangular lattice graphite by means of X - ray scattering in the range of 300 K - 950 K. The

value for the intertube gap is  $(4.2 \pm 1.4) \times 10^{-5}$  (1/K), which is larger than  $2.6 \times 10^{-5}$  (1/K) in graphite. The result reveals that nanotube has more lattice anharmonicity than that of graphite.

Chen *et al.* (2002) have investigated the room temperature x-ray diffraction which yields zero pressure bulk modulus values of  $K_{67} = 238 \pm 3$  GPa and  $K_{37} = 172 \pm 3$  GPa for nanocrystalline  $\gamma$ -alumina ( $\text{Al}_2\text{O}_3$ ) with particle size of 67 and 37 nm respectively. Under high pressure x-ray studies of 20 and 6 nm nanocrystal  $\text{Al}_2\text{O}_3$ , it is noted that the rigidity decreases with increasing the size of nanoparticle. A new phase is detected at pressure above 51 and 56 GPa for  $\gamma$ - $\text{Al}_2\text{O}_3$  of 67 and 37 nm respectively.

Mounet *et al.* (2005) used a combination of density-functional total energy theory and density-functional perturbation theory to investigate the thermodynamic characteristics of diamond and graphite. They discovered a good correlation between structural characteristics and phonon dispersions.

Kirtania *et al.* (2007) used 3D finite element analysis to investigate the young's modulus and co-efficient of thermal expansion (CTE) of single walled carbon nanotubes (SWCNT's) and graphene sheets (FEA). The following major observations have been made after analysing both arm chair and zigzag SWCNTs: The young's modulus of armchair and zigzag nanotubes rises as the size of the graphene sheets decreases, whereas it drops as the wall thickness of the nanotube decreases.

Yoon *et al.* (2011) used temperature dependent Raman spectroscopy to investigate the coefficient of thermal expansion (CTE) and strain of twisted graphene. They discovered that TEC remains negative throughout the temperature range of 200-400K and that there is a strain mismatch between graphene and its substrate.

Deepika Joshi *et al.* (2005) explore the thermo-elastic characteristics of close packed phases of copper and aluminum up to their melting temperatures. The characteristics are derived using the integral form of the equation of state (IFEOS), which was recently presented by Singh and Gupta and assumes that the Anderson parameter is constant. ( $\delta T$ ) strongly depends on temperature due to contribution from the thermal excitation of electrons. The values of thermal expansion ( $V/V_0$ ), thermal expansivity ( $\alpha T$ ) and bulk modulus (KT) as determined in the present study, agree closely with the data based on temperature-dependent experimental studies.

According to Heshmatpour and Aghakhanpour (2011) Synthesis and characterization of nanocrystalline zirconia powder by simple sol-gel method with glucose and fructose as organic additives," as the calcination temperature rises, the diffraction peaks become sharper and narrower, and their intensity rises noticeably, indicating a significant improvement in crystallinity of the  $\text{ZrO}_2$  nanocrystals.

## THEORETICAL REVIEWS OF NANOMATERIALS

Singh, *et al.* (2003) regarded the Anderson Gruneisen parameter to be temperature dependent and calculated the isobaric integral form of the equation of state.

K.Y. Singh, *et al.* (2003) used the Shanker equation of thermal expansivity to compute the volumes of  $\text{CaSiO}_3$ ,  $\text{MgSiO}_3$ ,  $(\text{Mg}_{0.9}\text{Fe}_{0.1})\text{SiO}_3$  and  $(\text{Mg}_{0.9}\text{Fe}_{0.1})\text{SiO}_3$  perovskites at high temperatures and pressures. The derived findings are found to be in close accord with recent experimental P-V-T data for the solids under consideration. The Anderson-Gruneisen parameter is found to vary dramatically at high temperatures, and the findings are altered. The current approach has been proven to be beneficial for estimating solid volumes at high temperatures.

Deepika Kandpal, *et al.*, (2004) "On pressure dependence on relative compression ( $V/V_0$ ) at room temperature for solids: copper and lead prototypes," the results obtained from this study from the modified Usual Tait's equation of state are found to be closer to the available experimental data than those values obtained without taking the correction factor into account in the original Tait's equation of state.

Bhagwat and Ramaswamy (2004) manufactured nanocrystalline zirconia powder by the amorphous citrate technique, noting that for zirconia, inter-atomic separation increased

with increasing temperature and that its stability into the tetragonal phase was owing to its tiny size.

Based on Mott's equation for the melting entropy and a model for the size-dependent melting temperature, Zhang, *et al.* (2005) proved that a simple model, devoid of any changeable parameters, can be built for the melting enthalpy and melting entropy of nanocrystals. The findings were validated by experimental data on metallic and organic crystals. It has also been proposed that the vibrational component of overall melting enthalpy and entropy can be used to calculate size dependent melting enthalpy and entropy for nonsemiconductor crystals.

Seeleboyina *et al.*, (2005) investigated high temperature micro x-ray diffraction on nanocrystalline and bulk samples of NiO, anatase TiO<sub>2</sub>, and ZnO. The bulk and nano sample values were determined to be 475K-1417K for NiO, 300K-883K for TiO<sub>2</sub>, and 300K-1426K for ZnO. According to the findings of this study, the volume thermal expansion co-efficient of nano crystalline NiO is greater than that of bulk NiO crystal.

Mounet *et al.* (2005) Using a mixture of theory, the density-functional total energy theory and density-functional perturbation thermodynamic characteristics of diamond and graphite were investigated. He discovered the optimal balance of structural characteristics and Phonon dispersion.

Hirvonen *et al.* (2006) concluded that ZrO<sub>2</sub> (zirconia) is a material of great technological importance, with good natural colour, high strength, transformation toughness, high chemical stability, excellent corrosion resisting material, and chemical and microbial resistance, in their paper "fabrication, structure, mechanical and thermal properties of zirconia-based ceramic nanocomposites."

Gole *et al.* (2006) investigated the "unique features of selectively generated zirconia nanostructures" and discovered that ZrO<sub>2</sub> is a broad band gap p-type semiconductor with many oxygen vacancies on its surface. Because of its strong ion exchange capacity and redox activities, it is helpful in catalysis.

Ulrike Troitzsch (2006) has also studied the phase transition behavior of ZrO<sub>2</sub> -TiO<sub>2</sub> system with the monoclinic-tetragonal phase transition with increasing Ti-content.

Qi, *et al.* (2006) established a model for the size-dependent and coherence-dependent cohesive energy, melting temperature, melting enthalpy, vacancy formation energy, and vacancy concentration of nanowires and nanofilms. The coherent interface determines the direction of variation (increasing or decreasing) of thermodynamic characteristics, and the quantity of variation relies on crystal size.

Roy (2007) investigated "nano crystalline undoped tetragonal and cubic zirconia manufactured utilizing poly-acrylamide as gel and matrix," and determined that ZrO<sub>2</sub> has three well-defined crystal phases, namely cubic (c-ZrO<sub>2</sub>), tetragonal (t-ZrO<sub>2</sub>), and monoclinic (m-ZrO<sub>2</sub>).

According to melting hypothesis, Chandra *et al.* (2008) discovered that the declining trend of bulk modulus with rising temperature. Chandra determined the elastic characteristics of diverse solids such as AgO, AuO, NiO, MnO, and alkali halides such as NaCl and KCl using the Singh and Gupta equation of state (IFEOS), such as volume thermal expansion, expansion coefficient, and bulk modulus.

Kovalenko *et al.* (2008) investigated the production of ZnO/NiO nanocomposites as a combination of two phases and detailed their phase relationship as the unit cell volume increased at different temperatures.

Chandra *et al.* (2008) investigated the thermal characteristics of nanomaterials such as n-ZnO, TiO<sub>2</sub> anatase, and n-NiO at high temperatures using the equation of state (IFEOS). The IFEOS is said to successfully describe the thermo-elastic characteristics of nanomaterials. Because of the high surface-volume ratio of nanoparticles, their thermal characteristics differ from those of bulk materials.

Using Singh, *et al.* (2009) estimated the thermal expansivity, thermal expansion, and bulk modulus of nanomaterials. They derived conclusions for these materials that forecast the



agreement with experimental data and also indicate the declining trend of bulk modulus with temperature that has been seen for bulk materials.

Safaei and Shandiz (2009) have studied the lattice type sensitive model for the melting entropy and enthalpy of nanocrystals, which is based on the model for size dependence of melting point. The formulations have been compared with experimental data of results and molecular dynamic simulation results of Ag nanoparticles.

Schiller *et al.* (2010) have studied the phase stability of Zr doped anatase at various concentrations using sol-gel method and its effect on the crystallinity and phase composition at various temperatures.

Kumar *et al.* (2011) studied the effect of temperature by an alternative method based on thermodynamics variables. They determined the effect of temperature on Zr, Ag, ZnO, NiO and Al composites by alternative method and reported a good agreement between theory and experimental.

Xiong *et al.* (2011) discussed that most thermodynamic properties of nanoparticles vary linearly with  $D^{-1}$  as first approximation. Thus, it seems that there exist some efforts to study the size dependence of melting entropy and enthalpy of nanoparticles. Moreover, these quantities also depend on the shape, which is a very important phenomenon of nanoscience.

Mahipal Singh *et al.* (2013) give a study on nanomaterials by using different equation of state and studied the thermal expansion of rock salt and wurzite phase of zinc oxide nanomaterials. It is stated by them that upto room temperature range the thermal expansion increases with slow rate in both the phases of zinc oxide while in high temperature range, however, the thermal expansion increases with high rate in rs-ZnO and slow rate in w-ZnO above room temperature.

Kumar *et al.* (2013) have studied the "effect of size and shape on the vibrational and thermodynamic properties of nanomaterials". The results obtained are compared with the experimental data. A good agreement between the model predictions and the experimental data supports the theory developed in the present paper.

Chandra *et al.* (2014) also described the comparative analysis of thermal expansion, thermal expansivity and isothermal bulk modulus of zinc oxide nanomaterials (w-ZnO&rs-ZnO) under high temperature. He used the equation of state described by various workers; however, the results obtained by them are not in good agreement with the experimental data.

Kuldeep Kholiya *et al.* (2014) have used the equation of state (EOS) to analyze the high pressure compression behavior of  $Zr_{0.1}Ti_{0.9}O_2$ . He assumed the pressure to quadratic expressions of relative volume and density changes. Their findings are in good accord with the experimental data and refute the Kumar equation, in which pressure is considered the second component of relative changes only in moderation.

Lee *et al.*, (2015) studied "A simple up-scalable thermal treatment method for synthesis of ZnO nanoparticles," and concluded that as particle size increases, so does the number of atoms that form a particle, making valence and conduction electrons more attractive to the ions core of the particles and thus decreasing the band gap of the particles.

Aysaret *al.* (2016) investigated the "structural and optical properties of zirconia nanoparticles by thermal treatment synthesis" and discovered that by eliminating the drying process (24 h) in the current thermal treatment method, size-controlled zirconia nanoparticles were conveniently manufactured with a reduction in synthesise time and energy consumption, making them suitable for large-scale fabrication.

Aguannoet *al.*, (2016) presented "structural and thermodynamic properties of nanomaterials for thermal energy storage at high temperature" and demonstrated a strategy for systematically designing nanofluids with enhanced CP, nf by combining a set of experimental techniques (DSC, adiabatic calorimetry, DLS, and SANS) and several cutting-edge simulation tools (classical and first principles MD).

Menjiao Li *et al.* (2016) investigated the "size dependence of surface thermodynamic characteristics of nanoparticles and technique of measurement using reaction rate

constant." As a consequence of discussing the effect regularities of particle size on the surface thermodynamic characteristics, they discovered that as particle size increases, the molar surface thermodynamic properties rise, but the surface heat capacity decreases. Furthermore, the surface thermodynamic parameters are directly proportional to the reciprocal of the nanoparticle diameter.

Cheng *et al.* (2017) investigated the influence of the dopant on the material electrical structure and the size of the mixed oxide nanoparticles with temperature variations in zirconia-titania mixed metal oxides at varied concentrations.

Qingshan Fu *et al.*, (2018) "Research of Size- and Shape-Dependent Thermodynamic Properties of the Actual Melting Process of Nanoparticles". They derived relations of melting thermodynamic properties can quantitatively describe the actual melting behaviors of nanoparticles, and the findings herein provide us a comprehensive understanding of the melting thermodynamic properties of nanomaterials in the whole melting process.

Barbara, *et al.*, (2019) His multifaceted seminal work in magnetism and obtained in ferrite spinel, according to Neel's two-sublattice model of ferrimagnetisms three types of magnetic interactions occur between sites A and B, namely A-A, B-B, and the strongest and most dominant A-B sub-lattice exchange.

Guisbiers (2019) used a top down approach and reported a universal relation, which is particularly helpful when experiments are difficult to lead on a specific material property. To validate the relation Guisbiers compared the theoretical relation with experimental data of cohesive energy of Mo and W nanoparticles and of activation energy of diffusion for Fe and Cu nanoparticles.

Dash *et al.*, (2019) studied "Impression of magnetic clusters, critical behavior and magnetocaloric effect in Fe<sub>3</sub>Al alloys" and resulted that the Ni-Zn-Al spinel ferrite can be considered as a candidate for magnetic refrigeration in a wide temperature range above room temperature and to transform industrial waste transformed into electrical energy using a thermomagnetic generator.

Gregory Guisbiers, 2019 have studied "advances in thermodynamic modelling of nanoparticles" In this review, they first introduce the fundamental concepts and methods of nanothermodynamics starting from Hill's contributions to the most recent developments focusing specifically on the relationship between the material property and the following parameters as quantum statistics (Fermi-Dirac or Bose-Einstein), size and shape of the nanoparticle.

Jalelmassoudiet *al.* (2020) studied "Magnetic and spectroscopic properties of Ni-Zn-Al ferrite spinel: from the nanoscale to microscale" and stated that the optical properties of synthesized NZFAO nanoparticles were investigated, and the differences caused by the particle sizes are discussed on the basis of the phonon confinement effect. This effect was also inspected by the Raman analysis. Tuning of the physical properties suggests that the Ni-Zn-Al ferrite samples may be promising for multifunctional diverse applications.

Rabi *et al.* (2020) investigated "Structural, magnetic, and magnetocaloric research of Ni<sub>0.5</sub>Zn<sub>0.5</sub>Fe<sub>2</sub>O<sub>4</sub> spinel," and discovered that the relationship between structures and physical characteristics for nano ferrites must be carefully considered. As a result, several techniques, such as forced hydrolysis in polyol, ball milling, coprecipitation, sol-gel auto-combustion, and hydrothermal/solvothermal processes, have been widely developed to produce nano-spinel ferrite of varied sizes and forms.

Das *et al.* (2020) investigated the relationship between coercivity (H<sub>c</sub>) and grain size. They discovered that for CoFe<sub>2</sub>O<sub>4</sub> nanoparticles, it increases first up to 40 nm and subsequently drops. The declining trend of H<sub>c</sub> with grain size greater than 40 nm suggests that a single domain particle is being transformed into a multidomain particle.

Lin Qiu and colleagues (2020) investigated "A review of recent achievements in thermophysical characteristics at the nanoscale: From solid state to colloids." They described current advances in theoretical, experimental, and computational techniques to

understanding and manipulating the thermophysical characteristics of solid-state to colloidal nanomaterials.

Termentzidis *et al.* (2020) investigated the interfacial geometry dependency of  $k$  for superlattices determined using EMD and NEMD simulations. If the MFP and superlattice period are of the same order of magnitude, superlattice thermal transfer is governed by height and roughness. In particular, the in-plane  $k$  is dominated by the height-to-roughness ratio and superlattice period, but the out-of-plane  $k$  rises monotonically owing to interfacial phonon scattering.

### EFFECT OF TEMPERATURE & PRESSURE ON NANOMATERIALS

The physical and chemical characteristics of nanomaterials are primarily determined by the surface area of grain boundaries, where a substantial number of atoms, around 80% of the total number, stay on the surface, as opposed to bulk materials, where only 15% to 20% of the atoms remain on the surface. Due to the grain boundaries and large surface-volume ratio in nanomaterials they show very different and anomalous behavior under high temperature and high pressure as compared to their counterpart bulk materials. The strength and elastic properties of such materials also depend upon the inter-atomic bonding between the atoms. Under high pressure and high temperature the nanomaterial structure is generally changed and transform to different phase structure because of the change in inter-atomic separation between the grains remain at the boundary of the material. This is why the nanomaterials show the anomalous behavior under high pressure and high temperature.

The temperature and pressure dependent characteristics of nickel (n-Ni) metal have piqued the curiosity of many researchers in recent years Bonetti *et al.* (1998), Valiev *et al.* (1997), Chain *et al.* (2000). Nickel is a transition ferromagnetic 3d metal that is commonly employed in harsh settings as a catalyst. The grain boundaries structure has been extensively researched to better understand the characteristics of nickel using transmission electron microscopy (TEM), X-ray diffraction (XRD), and inelastic neutron scattering methods. The study of graphene's thermo-mechanical characteristics has also piqued the interest of researchers due to its prospective uses in electronic materials Geim (2009), Bonaccorso *et al.* (2010) and Ph. Avouris *et al.* (2010) as well as its extraordinary features Peres (2010), Novoselov *et al.* (2005) and Zhang *et al.* (2005). Because of its excellent thermal conductivity and exceptionally high mechanical strength, it is a promising candidate material for heat regulation in electrical equipment. Experiments reveal that the strain of a grapheme sheet put on a substrate is substantially greater than that of graphene hanging in air. The thermo-physical characteristics reported in compressing and stretching tests were anticipated by two primary theoretical models based on thermo-elastic theory and empirical inter-atomic potentials Frank *et al.* (2010), Zhakharchenko *et al.* (2009) and Neck-Amal and Peeters (2010). It should be highlighted that the elastic theory does not provide atomic aspects of graphene, but empirical potentials such as the Brenner potential Brenner (1990) and Brenner *et al.* (2002) valence force and the LCBOPII potential Los *et al.* (2005) may correctly account for graphene's thermo-elastic properties.

### CONCLUSION

Nanomaterials have a lengthy history, and humans have inadvertently used them. Feynman's renowned address "There's Plenty of Room at the Bottom" introduced the notion of contemporary nanotechnology to academia. Following this, there has been significant development in nanotechnology, and the subject is constantly spreading into new domains. Materials are typically called nanomaterials if their dimensions fall between 1 and 100 nm. Nanomaterials have exhibited a number of different features that set them apart from their bulk counterparts. Nanomaterials have a huge surface area, are magnetic, exhibit quantum effects, are antimicrobial, and have good thermal and electrical conductivities. Metal-based materials have shown very high catalytic activity at the



nanoscale, and enhanced dispersion of these catalysts may be produced by dispersing them over 2D sheets of other nanomaterials, therefore improving the overall performance of metal-based catalysts. In biomedical applications, synthetic nanoparticles such as Abraxane and Doxil are used. These nanoparticles have been approved for use in clinical studies as medications. Submicron TiO<sub>2</sub> particles are a key ingredient in white paints. Commercial sunscreens comprise zinc oxide and titanium dioxide oxide nanoparticles. Smijs and Pavel (2011) is generated in huge quantities on an industrial scale every year. In commercial LCDs, colour pigments with crystal sizes smaller than 40 nm are utilised to increase colour purity, brightness, and contrast for high-definition television-based applications. Stark *et al.* (2015) Aside from a few examples, most nanomaterials are being created for lab-scale applications, and major efforts will be required to get them to the commercial market. Another key challenge associated with contemporary nanotechnology is the discovery of alternatives to the use of endangered and limited-resource materials in the production of nanomaterials. In the coming years, 44 elements out of 118 will face supply shortages. Precious metals, phosphorus, and rare-earth elements are examples of critical elements. There is an urgent need to reduce reliance on vulnerable and critical components. In batteries, for example, efforts are being made to substitute crucial lithium ions with more abundant metal ions. Because carbon sources are widely available, carbon-based nanomaterials are an attractive choice for large-scale synthesis for a wide range of applications. Core shell morphologies can also help to reduce the consumption of critical components in a range of applications. Water purification and wastewater recycling have the potential to benefit from nanotechnology. Future challenges affecting contemporary civilization can be handled with greater knowledge and the fast rise of nanotechnology. Furthermore, there is still room to research the thermo-physical characteristics of nanoparticles for which no suitable materials exist. Model theory could provide the satisfactory results under the effect of high temperature and high pressure.

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