

Analysis of Mechanical Properties Of Nano Molybdenum And Nano Nickel Using High Pressure Equation of State

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Abstract

In the present paper we have studied high pressure behaviour of nano crystalline molybdenum of particle size 100nm, and nano nickel of two different particle sizes 62 nm and 20 nm together with its bulk counterpart using modified Tait's isothermal equation of state. In the present work the usual Tait's equation of state has been modified to predict the high pressure behaviour of nano materials. The results obtained in the present study are compared with available experimental evidences. Polynomial fit for the predicted values of bulk modulus for nano size samples along with their corresponding counterparts are computed in the present work. Our results on the study of compressibility show that nano size samples are less compressible than bulk materials which are in agreement with the Hall-Petch effect.

Keywords: Equation of state, nano crystalline materials, compressibility.

Introduction

Over the past decade, nanomaterials have been the subject of enormous interest. These materials, notable for their extremely small size, have the potential for wide-ranging, bio-medical and electronic applications. Nanomaterials can be metals, ceramics, and polymeric materials, nanocrystalline materials with particle size of 1-100 nm are of current interest because they show noble physical and chemical properties that may differ from those of the corresponding bulk materials. Compared

with bulk materials, nanocrystalline materials have larger surface to volume ratio, fewer dislocation, and lattice relaxation at grain boundaries. LI Xiao-Dong et al.[1] have reported numerous investigations on differences between the bulk and nano materials in the physical, electronic, and magnetic properties. H. Wang et. al [2] suggested that the value of bulk modulus decrease with decreasing grain size for Fe, Cu, Al₂O₃ and PbS. On the other hand, the bulk modulus increases with decreasing grain size for nanocrystalline TiO₂, CeO₂, AlN, ZnS:Eu and γ -Fe₂O₃, whereas the bulk modulus of the nanocrystalline material is similar to that of the large-grained sample for Ni, ϵ -Fe and CuO.

Numerous experimental and theoretical work has been done on molybdenum and nickel due to their simple structure and stability at extreme pressures and temperatures [3]. Molybdenum is a bcc 4d transition metal whose properties are interesting in number of aspects. Its high pressure behaviour has received a lot of interest as molybdenum is one of the elements forming the basis of ultra high pressure scale and was used in the calibration of the ruby-fluorescence pressure scale [4]. Equation of State of bcc Mo was computed theoretically and found to agree very well with experimental data [5]. X-ray diffraction studies of nano molybdenum were conducted by Selva Vennila. R et al. [3] to understand its high pressure behaviour.

Nickel is an important ferromagnetic 3d metal belonging to the eighth group and third period. Iron-nickel alloy is the most abundant component in the earth's core. As a vital alloying constituent of stainless steel, nickel plays a key role in the industries. There are several experimental and theoretical studies on nanocrystalline nickel that contradicts each other when describing its compression behaviour under pressure as a function of particle size. Xiaogang J. et. al [6] studied the equation of state of nano and bulk nickel and suggested that nano nickel is more compressible than bulk nickel, whereas Chen B. et. al [7] measured the compressibility of nano nickel of size 20 nm and reported that bulk modulus did not vary with particle size when compared to theoretical results.

In the present work we are analysing the mechanical properties especially the volume compression and the bulk modulus of nano molybdenum of particle size 100 nm and nano nickel of two different particle sizes 62 nm and 20 nm together with their bulk counterparts, using modified Tait's equation of state.

Method of Analysis

The usual Tait's equation of state is obtained by assuming the fact that the product of the thermal expansion coefficient α and the isothermal bulk modulus B remains constant under the effect of pressure [8].

$$\alpha B = \text{constant} \quad (1)$$

Differentiating eqn. (1) with respect to volume at constant temperature, we get

$$\alpha \left(\frac{dB}{dV} \right)_T + B \left(\frac{d\alpha}{dV} \right)_T = 0 \quad (2)$$

δ_T is known as Anderson-Gruneisen parameter at constant temperature which is defined as:

$$\delta_T = \frac{V}{\alpha} \left(\frac{d\alpha}{dV} \right)_T \quad (3)$$

Assuming δ_T to be independent of V

$$\delta_T = \left(\frac{dB}{dP} \right)_T = B'_0 \quad (4)$$

$$B = -V \left(\frac{dP}{dV} \right)_T \quad (5)$$

We get the following final form of usual Tait's equation of state [9].

$$\frac{V(P, T_0)}{V(0, T_0)} = 1 - \frac{1}{B'_0 + 1} \ln \left[1 + \left(\frac{B'_0 + 1}{B_0} \right) P \right] \quad (6)$$

Where, $V(P, T_0)$ is the volume of the solid at pressure P required to compress it, keeping the temperature constant. $V(0, T_0)$ is the initial volume at $P = 0$ at reference temperature T_0 . B_0 and B'_0 are the isothermal bulk modulus and its first order pressure derivative at zero pressure. The above isothermal equation of state can be also written as

$$P = \frac{B_0}{(B'_0 + 1)} \left[\left\{ \exp(B'_0 + 1) \left(1 - \frac{V(P, T_0)}{V(0, T_0)} \right) \right\} - 1 \right] \quad (7)$$

Expanding the exponential term in eq. (7) and including the third order term we get the following modified Tait's equation of state

$$P = B_0 \left[\left(1 - \frac{V}{V_0} \right) + \left(\frac{B'_0 + 1}{2} \right) \left(1 - \frac{V}{V_0} \right)^2 + \frac{(B'_0 + 1)^2}{6} \left(1 - \frac{V}{V_0} \right)^3 \right] \quad (8)$$

The special feature of this equation of state is that it requires less number of input parameters and provides a simple and straight forward approach to predict the high pressure behaviour of solids. In principle, the isothermal bulk modulus B_T can be determined from an isothermal equation of state representing the relationship between pressure and volume at fixed temperature. The bulk modulus derived from eq. (6) is given as

$$B = B_0 \left(\frac{V}{V_0} \right) \left[1 + \left(\frac{B'_0 + 1}{B_0} \right) P \right] \quad (9)$$

Tait's equation of state is found to be in extensive use to all kinds of solids at high pressure. In the present work we have applied the modified Tait's equation of state for nano crystalline molybdenum and nickel to predict their high pressure behaviour and verified its validity for nano materials.

Results and Discussion

The input parameters required for the analysis of mechanical properties of nano molybdenum and nano nickel compiled from Selva Vennila. R et al. [3] are given in Table 1. The compression behaviour of nano molybdenum and nano nickel using modified Tait's equation of state along with their experimental findings [3] are

reported in Fig. 1 and Fig. 2 respectively. The predicted results are found to be in good agreement with the experimental data for both the cases. Compression behaviour of nano molybdenum and nano nickel along with their bulk counterparts are shown in Fig. 3 and Fig. 4 respectively. It is clear from both figures that nano molybdenum and nano nickel are less compressible than their bulk counterparts. In Fig. 5 and Fig. 6, we report the variation of the bulk modulus for nano molybdenum and nano nickel and their bulk counterparts against pressure and it is observed to be increasing with increasing pressure. Bulk modulus for the nano size samples shows a higher value when compared to that of bulk samples in both systems.

By fitting the calculated data of bulk modulus to a third order polynomial we obtain following relationships for nano molybdenum and nickel and their corresponding bulk counter parts.

For molybdenum

$$B_T(\text{bulk}) = 261 + 4P - 0.0095P^2 + (4.8 \times 10^{-5})P^3$$

$$B_T(100\text{nm}) = 273 + 3.78P - 0.0086P^2 + (3.7 \times 10^{-5})P^3$$

Similarly for nickel,

$$B_T(\text{bulk}) = 180 + 4P - 0.014P^2 + (1.0975 \times 10^{-5})P^3$$

$$B_T(62\text{nm}) = 216 + 4P - 0.0116P^2 + (7.818 \times 10^{-5})P^3$$

$$B_T(20\text{nm}) = 228 + 4.02P - 0.0111P^2 + (7.11 \times 10^{-5})P^3$$

Conclusion

Our results on the study of compressibility of nano molybdenum and nano nickel shows that nano size samples are less compressible than bulk material, which is in agreement with the Hall-Petch effect [10]. Our result indicates that compressibility decreases with decrease in particle size, which may be the effect due to the larger surface between grains in nano sized particles that provides energy leading to the increase in their hardness.

Table No. 1

Material	Reference Temperature (K)	Bo (G Pa)	Bo'
Bulk Molybdenum	300	261	4
Nano Mo (100nm)	300	273	3.78
Bulk Nickel	300	180	4
Nano Ni (62 nm)	300	216	4
Nano Ni (20nm)	300	228	4.02

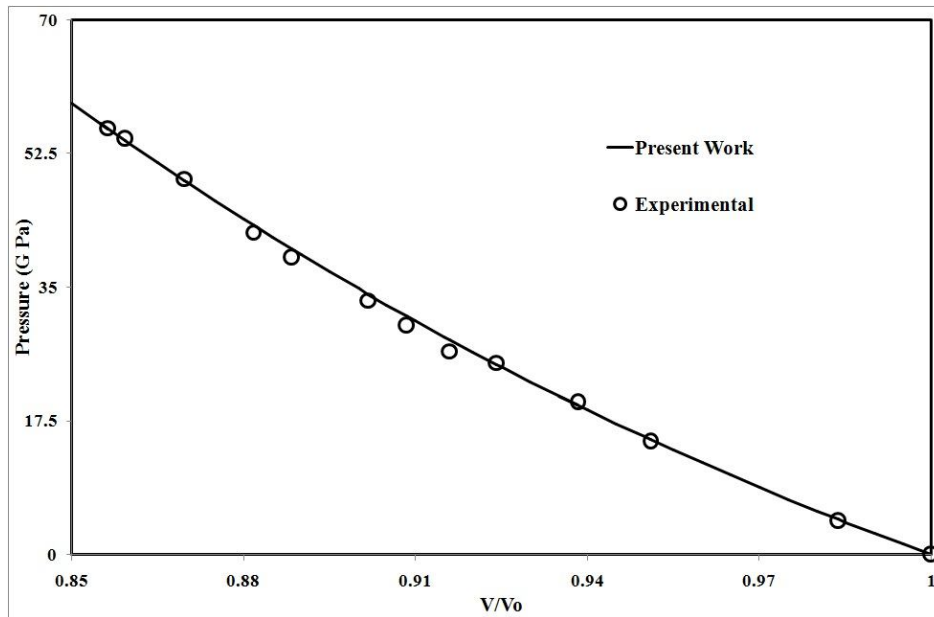


Figure 1 : Compression Behaviour of nano molybdenum (100 nm) along with the experimental P-V data.

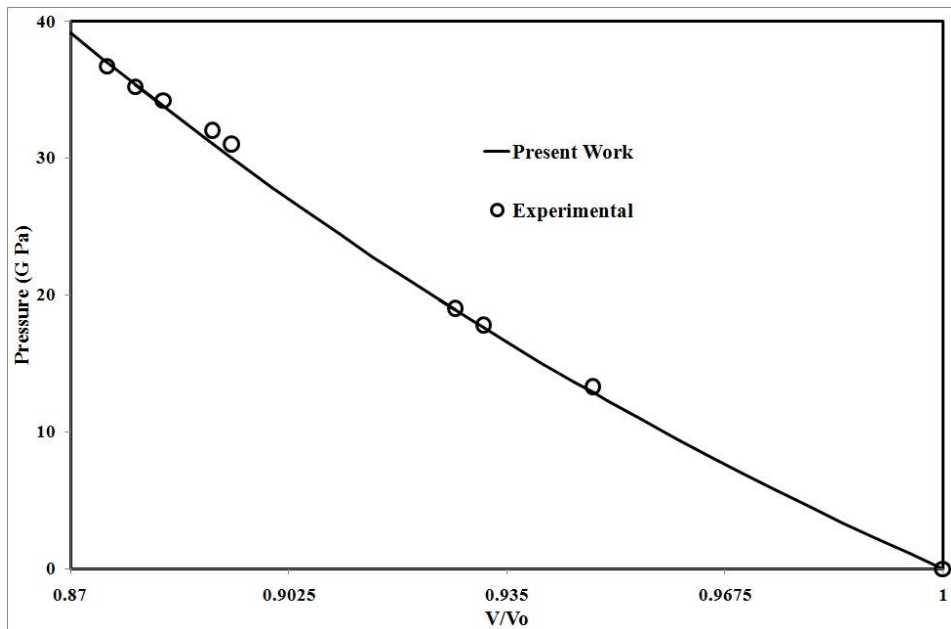


Figure 2 : Compression Behaviour of nano nickel (62 nm) along with the experimental P-V data.

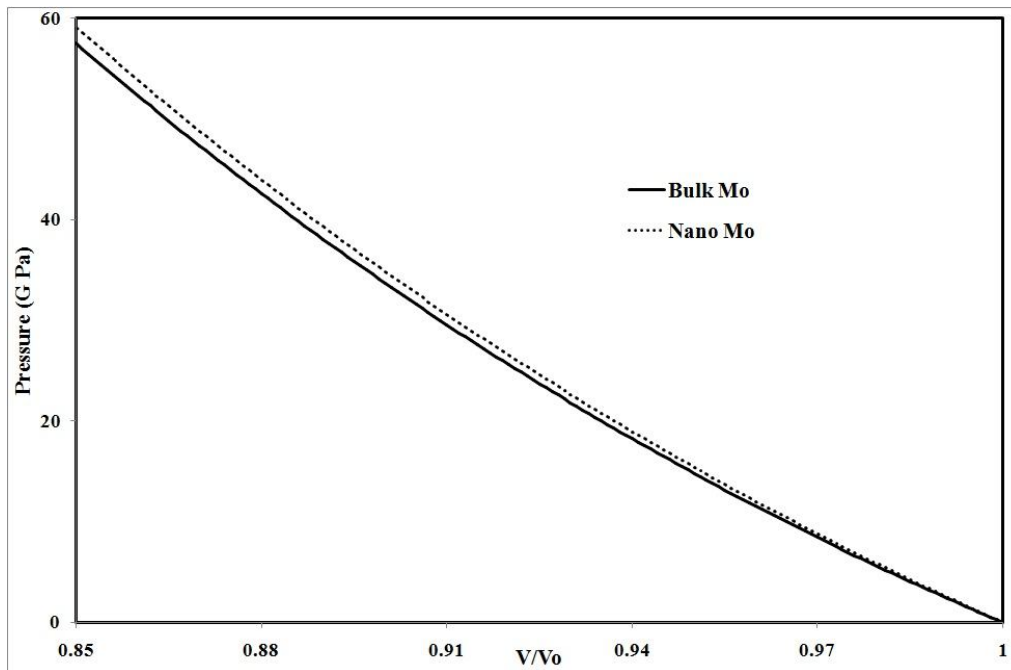


Figure 3 : Comparison of compression behaviour of nano molybdenum with its bulk counterpart.

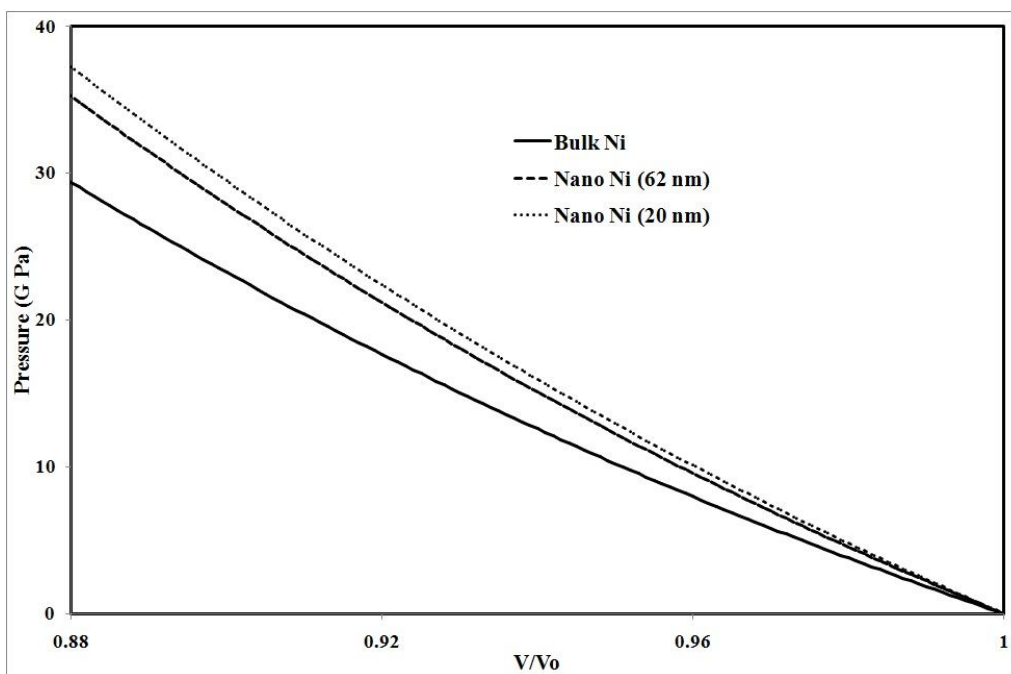


Figure 4 : Comparison of compression behaviour of nano nickel of two different particle sizes with its bulk counterpart.

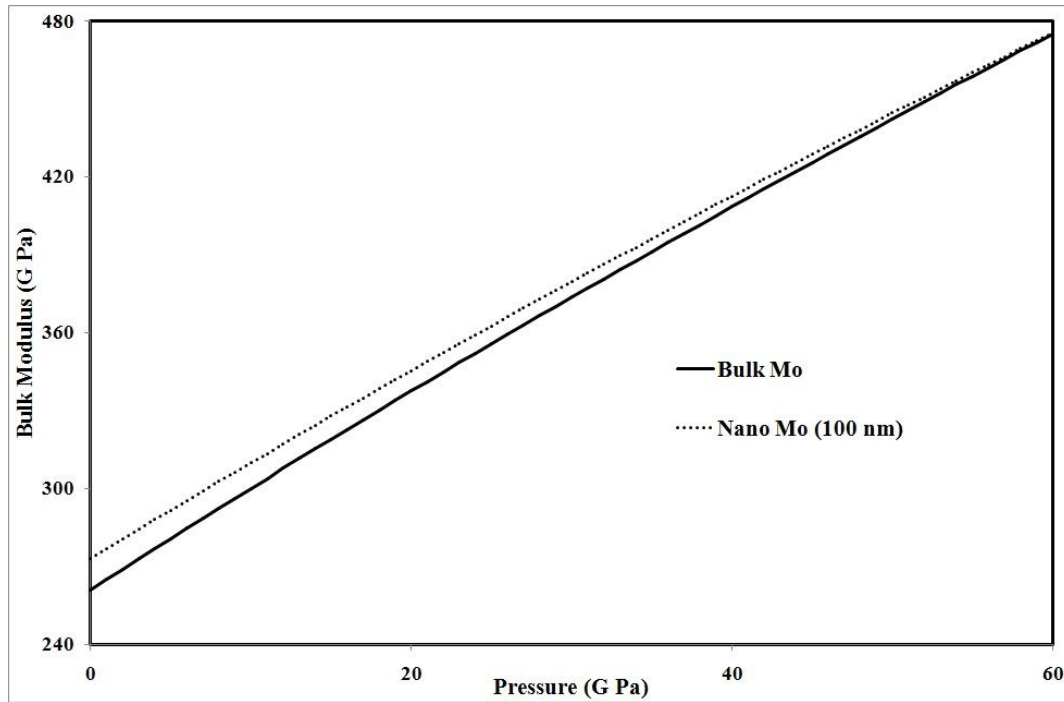


Figure 5 : Bulk Modulus versus pressure for nano molybdenum along with its bulk counterpart.

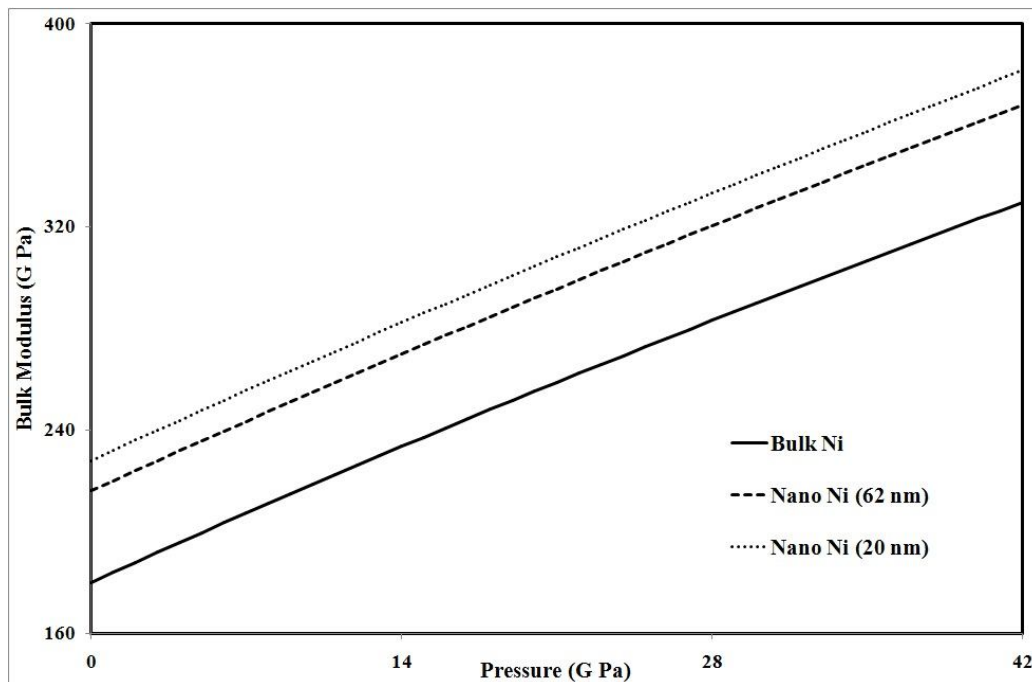


Figure 6 : Bulk Modulus versus pressure for nano nickel of two different particle sizes along with its bulk counterpart.

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