Modeling the quantitative effects of size, dimensionlity and temperature on Young's modulus of nanocrystals

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♦ Introduction

Nanocrystals have emerged as attractive candidates for aerospace, biological medicine, electronic devices, chemical catalytic, and other fields, due to their unique mechanical, physical, and chemical properties.

Space shuttle

nanoprobe

artificial intelligence

Sedan car

Notebook computer

♦ Theoretical model

Firstly, a new model was developed to comprehend the influences of size and dimensionality on cohesive energy by considering the surface stress and size dependent on surface energy, and it can be expressed as follows:

$$\frac{E_c(D,d)}{E_c(\infty)}=\frac{1-\dfrac{4(3-d)h\left[\dfrac{(3-d)S_{vib}(\infty)H_m(\infty)V_m(\infty)B}{2R}\right]^{\frac{1}{2}}}{3DE_c(\infty)\eta}}{1+\dfrac{(3-d)h}{3D\eta}}$$

Next, based on the solid state physics and Lennard-Jones potential, and further introduced the relationship between cohesive energy and average coordination number, as well as the size dependent on atom distance in equilibrium. The size and dimensionality effects on Young's moduls of nanocrystals can be given as:

$$\frac{Y(D,d)}{Y(\infty)}=\frac{E_c(D,d)/E_c(\infty)}{Z(D,d)/Z(\infty)}\Big/\left[\frac{h(D,d)}{h(\infty)}\right]^3$$

***Z*(*D*, *d*):**

$$\frac{Z(D,d)}{Z(\infty)}=\left[-1+\sqrt{1+8\frac{E_c(D,d)}{E_c(\infty)}}\Big/2\right]^2$$

***h*(*D*, *d*):**

$$\frac{h(D,d)}{h(\infty)}=1-\frac{4h}{3D}\sqrt{\frac{S_{vib}(\infty)H_m(\infty)(3-d)}{2BRV_m}}$$

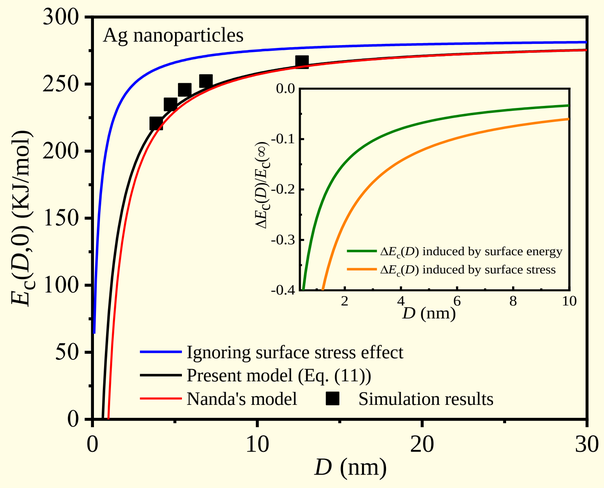
Finally, based on the above, and further considered the temperature dependent on cohenisve energy, atom distance in equilibrium, thermal expansion coefficient, and specific heat at constant volume, the size, dimensionlity and temperature effects on Young's modulus of nanocrystals can be expressed as:

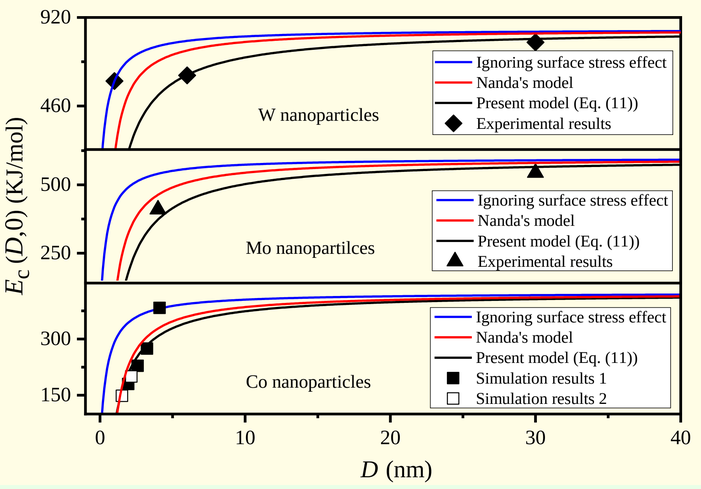
$$\frac{Y(D,d,T)}{Y(D,d,T_0)}=\frac{E_c(D,d,T_0)-\int_0^T C_V(D,d,T)dT}{E_c(D,d,T_0)\left[1+\int_{T_0}^T\lambda(D,d,T_0)dT\right]^3}$$

$$\frac{Y(D,d,T)}{Y(\infty,T)}=\frac{\dfrac{E_c(D,d,T)-\int_{T_0}^T C_V(D,d,T)dT}{E_c(\infty,T)-\int_{T_0}^T C_V(\infty,T)dT}}{\left\{\dfrac{h(D,d,T_0)\left[1+\int_{T_0}^T\lambda(D,d,T)dT\right]}{h(\infty,T_0)\left[1+\int_{T_0}^T\lambda(\infty,T_0)dT\right]}\right\}^3}$$

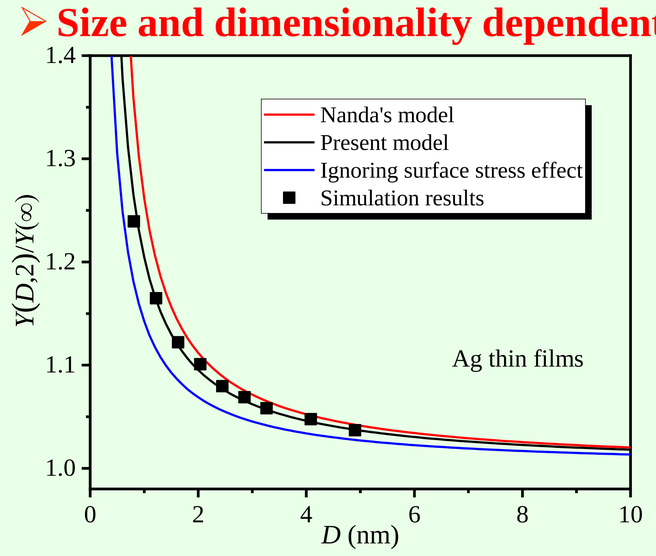
♦ Model Verfication

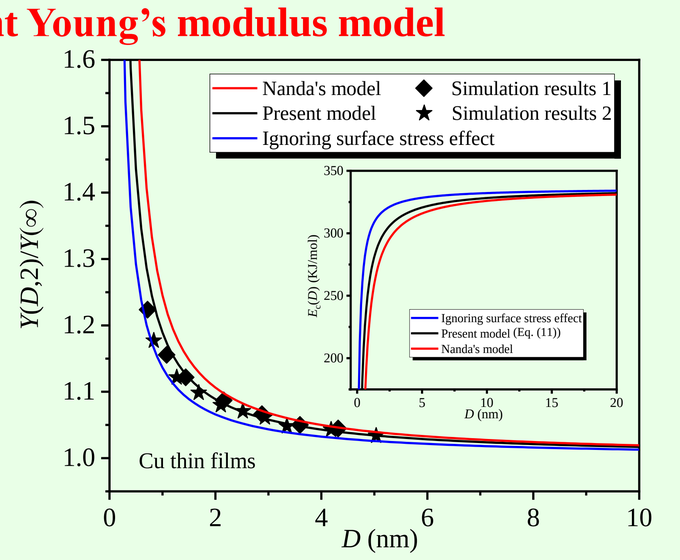
➢ Size and dimensionality dependent cohesive energy model

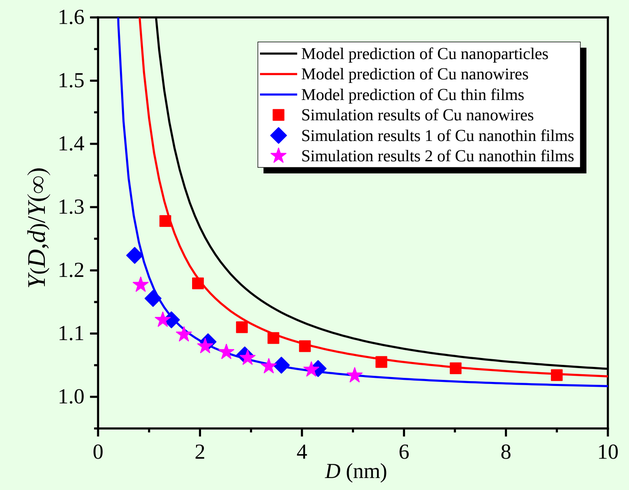


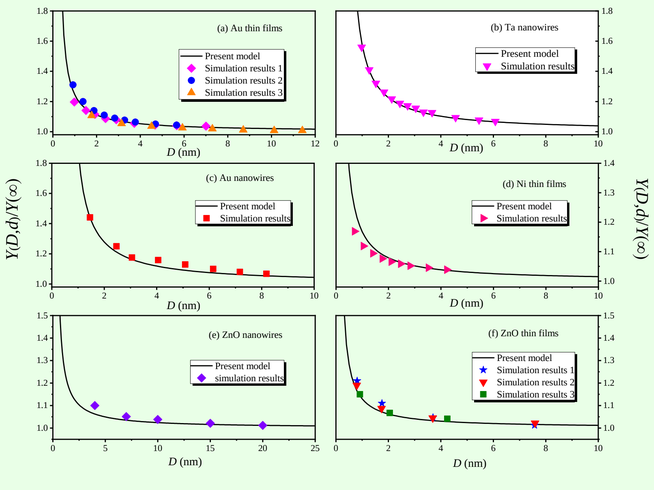


➢ Size and dimensionality dependent Young's modulus model

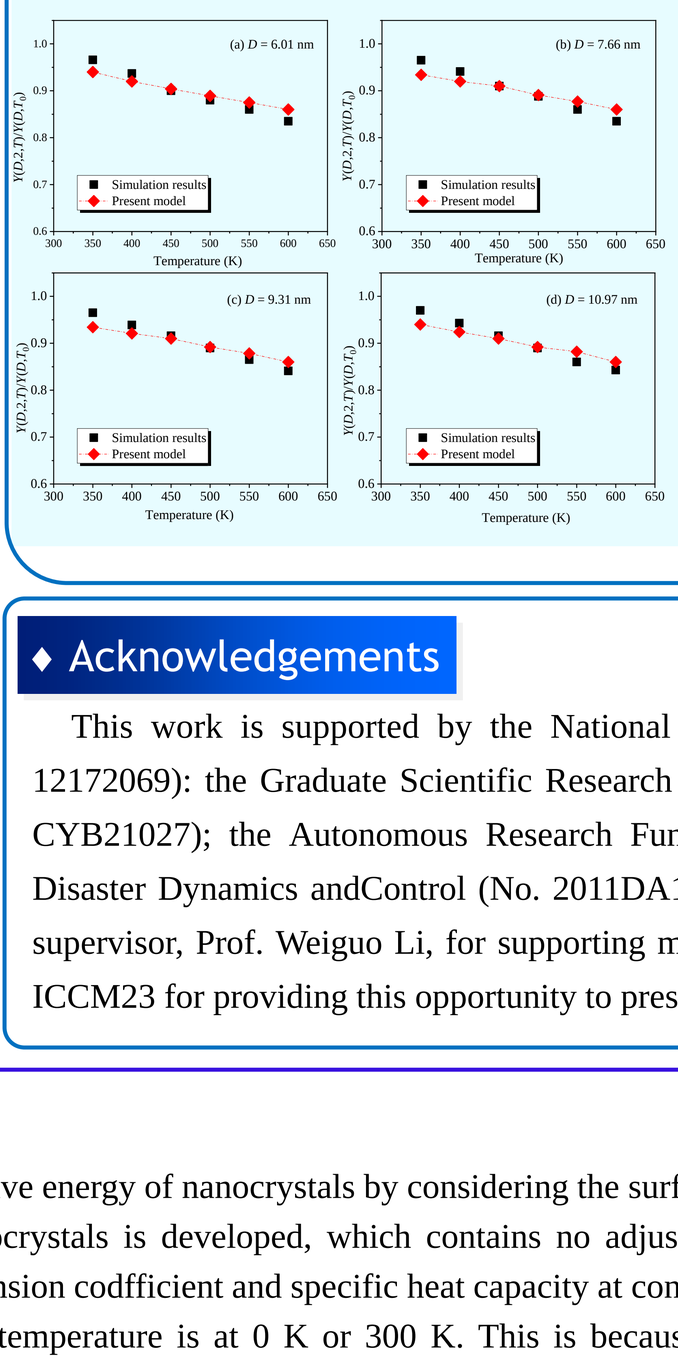


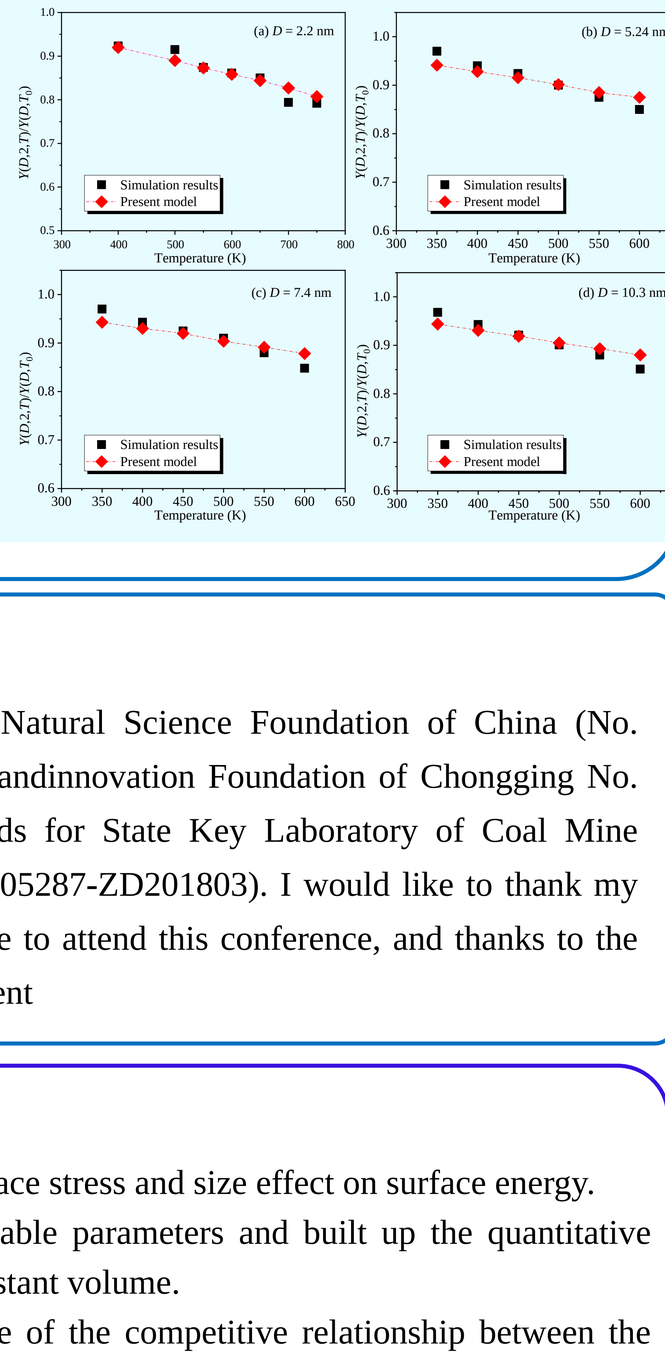






➢ Size, dimensionality and temperature dependent Young's modulus model





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♦ Conclusison

➢ A model is established to characterize the size and dimensionlity effects on cohesive energy of nanocrystals by considering the surface stress and size effect on surface energy.

➢The size, dimensionality, and temperature effects on Young's modulus of nanocrystals is developed, which contains no adjustable parameters and built up the quantitative relationship among Young's modulus, cohesive energy, atom distance, thermal expansion codfficient and specific heat capacity at constant volume.

➢Young's modulus increases or decreases with the decreasing of size when the temperature is at 0 K or 300 K. This is because of the competitive relationship between the enhancement and the reduction in Young's modulus by bond contraction and thermal stability decline.