Strength of nano ceramics with diamond like structure

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Materials on the basis of the light elements with covalent compounds have a set of valuable performance properties and also are suitable for creation of ceramic materials for various purposes. In the work by computational experiments are investigated nanoceramic materials - SiC, BN, AlN with cubic structure. It is assumed that the entire volume is filled with nanoceramical nanoplates, and the free surface of the grain is virtually absent, there are only the interfaces of grains. The objective of this study - construction (on the basis of an apriori pseudo potential) analytic model that adequately describes the mechanical properties of nanoceramics given as an interface between the grains. We believe that the nanoparticles have a diamond-like crystal structure and describe them in hexagonal axes, selecting for the Z-axis spatial diagonal of a cube [111]. The structure of the particles in this case is represented by a three-layer alternating close-packed atomic planes. As models we use a set of nanoceramical nanoplates with thickness *d* having a finite number of basal planes and Z spatial axis of which form angles $0 \le \alpha_l \le 90^0$. To describe the process of deformation of nanoceramics under uniaxial loading along the [111] proposed to use the value of the energy of interaction between neighboring atomic planes (perpendicular to the loading axis) [1]. In the ideal case (endless material sample along three coordinate axes), the energy of interaction between these structural units is Φ_0. Structural unit consists of two strongly coupled parallel close-packed atomic planes, which are separated by a distance *c*/12 (*c* – lattice parameter of tested material in hexagonal axes perpendicular to the basal plane). The interaction energy of the atomic planes in the i-nth layer of nanoplate considering interface has the following form [2]

$$\Phi_i = \Phi_0 - \Phi_0 \left(\frac{1}{2^{i+1}} - \frac{1}{2^{j+2-i}} - \frac{1}{j \cdot 2^j}\right)(\cos(\alpha_1) + \cos(\alpha_2))/2, \tag{1}$$

where *j* - the number of close-packed atomic layers in nanoplates, α_1, α_2 angles that form the atomic planes of neighboring nanoplates (top and bottom) with the atomic planes of selected nanoplates. To determine the average value of the nanoplate energy summarize (1) for all layers and divide by the number of layers (*j=3 d/c*). As a result, we obtain $\overline{\Phi} = \Phi_0 (1 - K_P \cdot 0{,}5\, d^{-1})$, where the Hall-Petch coefficient $K_P = \frac{c}{3}(2 - \frac{1}{2^{3d/c}})$ [3].

For known values of the interaction energy the strength is determined from the ratio $\sigma_C = \frac{1}{h}\frac{\partial \overline{\Phi}_P(h)}{\partial e_c}$, where e_z - relative deformation (deformation axis is perpendicular to the basic atomic planes); $\overline{\Phi}_P(h)$ - the average energy of interaction between two close-packed atomic planes separated by a distance h. The average peel strength nanoceramics represented as

$$\overline{\sigma}_C = \sigma_{0} (1 - K_p \cdot 0{,}5 \cdot d^{-1}), \tag{2}$$

where σ_0 - theoretical strength of the bulk crystal in the direction [111]. In case of $d \to \infty$ from (2) should that the strength of the material tends to its maximum value - the theoretical strength(σ_0) and that the nanoceramics strength is always greater than the strength of components grains (nanoplates) for which $\overline{\sigma}_p = \sigma_{0} (1 - K_p \cdot d^{-1})$. As a result of the quantum-mechanical calculations we get reverse Hall-Petch law for nanoceramics considering interface of grains.

1. *Zakarian D.A., Kartuzov V.V.* Calculation of the theoretical strength of diamond-like materials based on the interaction energy of the atomic planes // Reports of the NAS of Ukraine, 2006.- № 7.- p. 94-99.

2. *Zakarian D.A., Kartuzov V.V.* Simulation of influence of the scale factor on the theoretical strength of nanoparticles with a diamond-like structure // Reports of the NAS of Ukraine – 2008. - №2. – p.101-108.
3. *Zakarian D.A.,* Nanoparticles with a diamond-like structure and inverse Hall -Petch law // Reports of the NAS of Ukraine –2014.- № 19. –p. 82-86.