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Hall-Petch law for nanoparticles with diamond-like structure

Zakarian D.A., Kartuzov V.V., Khachatrian A.V.

IPMS National Academy of Science of Ukraine, Frantzevich Institute for Problems of Materials Science, Kiev-142, Krzhizhanovski st., 3. Ukraine E-mail: dora_zakaryan@mail.ru

For nanomaterial's with a grain size of several tens of nanometers Hall-Petch (H-P) law is violated, and manifests so-called inverse H-P effect, which mechanisms are currently poorly understood. Promoting understanding can give computer experiment based on ab initio calculations at the atomic level. Structure of nanoparticles with a diamond-like structure will be described in hexagonal axes, selecting for the Z-axis spatial diagonal of the cube [111]. The structure of the particles in this case will be described by three layers alternating of densely-packed atomic planes. The interaction energy between the atomic planes calculated within the aprioristic pseudopotential method, using interatomic potentials [1]. In this paper we show that the material is destroyed on the interlayer space, where the distance between atomic planes is c/4. We introduce the concept of structural units - two strongly coupled atomic planes at a distance c/12 from each other. Then the nanoparticle can be represented as a set of parallel structural units that are apart at a distance c/4. Assuming that the outer surface of the nanoplates has energy equal to half of the interplanar interaction energy, we can calculate the energy of interaction of atomic planes for nanoparticles [2], and through it, the theoretical strength. If nanoparticle has the same dimensions in three directions (d), the average value of nanoparticles strength will be $\langle\sigma_n\rangle = \sigma_0(1 - K d^{-1})$; $K = 2c/3 + 7.896a$. Here σ_0 – the theoretical strength, a, c - lattice parameters. The resulting formula essentially expresses the H-P law, not only for the polycrystalline material, and for perfect crystals in the transition to nanoscale volumes. Derived from first principles - the so-called inverse H-P law, where the dependence on the particle size is represented as d^{-1} instead $d^{-1/2}$. Hall - Petch factor K depends on the crystal lattice parameters, so for different crystals will have different values, as confirmed experimentally.

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