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Theoretical and real ultimate strength of crystals

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For nanomaterials with a grain size of tens of nanometers, the growth of the material’s strength limit with a decrease in the grain size is broken, and the opposite effect begins to appear. The task of this study is to describe the relationship between the values of theoretical strength and the ultimate strength of crystals. We consider nanoparticles with close-packed atomic planes perpendicular to the axis of deformation. For such a case, the dependence of the strength on the size of d0 (the size of the base) has the following form d0 =0 (1-k0d0-1).

The coefficient *к*0 depends on the parameters of the crystal lattice of the materials under study. For diamond-like materials for metals with fcc structure  In the case of real crystals, with a certain density of dislocations, the Hall-Petch law has the next form

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where \* is the ultimate strength for a given dislocation density for bulk materials. We measure the strength of the material, with a known dislocation density, which has an "unlimited" size. We reduce the size of the material (leaving the dislocation density constant) to a certain size, where the strength reaches its maximum value and then falls off. In parallel, we will calculate the strength of nanoparticles depending on their size. We find the size of the nanoparticle at which the value of the calculated strength is close (or coincides) with the strength values from the experiment



Finally, we obtain the relation

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Because the theoretical strength is a constant characteristic of the ideal structure, then the yield strength can be estimated at known values of *k0, k1* and *d0, d1*. The limiting strength of a diamond with a cubic structure and nickel is estimated, assuming that: *k0 = k1* and *d0 = d1 = 4 nm* (Tab.).

Tab. Theoretical and ultimate strength

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | Theoret. strength, GPa | | Ultimate strength, calculation | | ultimate strength, experiment.\* | |
| Stretching | Compression | Stretching | Compression | Stretching | Compression |
| Diamond | 100 | 204 | 6,17 (GPa) | 12,6 (GPa) |  | 8,9-12,9 (GPa) |
| Ni | 19,8 |  | 512 (MPa) |  | 400-500 (МPа) |  |

\* Handbook, Physical properties of diamond-Kiev, 1987, N.V. Novikov, Reference Chemistry of the 21st Century-Moscow 2015

There are good coincidences between the calculated and experimental values of ultimate strength (Tab). For more accurate calculations, it is necessary to determine experimentally the values of the coefficients k1 and the critical size of the grain d1.

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