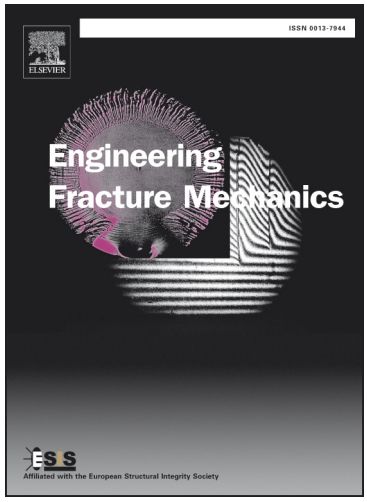

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Atomic mechanisms governing upper limit on the strength of nanosized crystals

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Abstract

The goal of this research is to present ideas on mechanisms governing the strength of nanosized crystals (NSC) and to estimate on this basis maximum attainable for them levels of strength. Findings of experimental measurement of strength of metallic nanoneedles and carbyne (*one-dimensional* carbon crystal, which strength two times exceeds strength of graphene) are also presented. Based on the results of MD-simulation and *ab-initio* calculations, it is exhibited that local instability of the lattice is the main mechanism governing the magnitude of strength of defect-free NSC, it temperature dependence and size effect. Regularities of dimensionality effect (growth of strength at transition from 3D to 2D and 1D crystals) are obtained and it explanation is given.

Keywords: nanocrystals; graphene; carbyne; upper strength limit, nanopillars.

1. Introduction

According to the existence paradigms of strength, there are two ways to increase strength, namely: (i) by increase in the density of defects in crystal lattice, other words – by increase a lattice distortion; or, vice versa, (ii) by creation of defect-free crystals. The first way is a classic approach to the manufacture of "ordinary" bulk materials. "Whiskers" are a classic representative of defect-free materials. Recently, nanotechnologies enable us to obtain defect-free nanocrystals (nanoneedles and nanopillars), as well as low-dimensional clusters – nanotubes, graphene, carbyne. Strength of these objects is much higher than those of conventional "bulk" materials and approaches to ideal strength of material. This extremely high strength of nanocrystals is directly used in nanodevices predetermining their strength and life-time. In addition to this traditional function of strength, specific feature of mechanical properties in nano-world is that in many cases they pre-determine the possibility of realization of functional

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