THE INFLUENCE OF GRAPHENE SLICES ON THE MECHANICAL PROPERTIES OF MONO- AND POLYCRISTALLINE α-IRON

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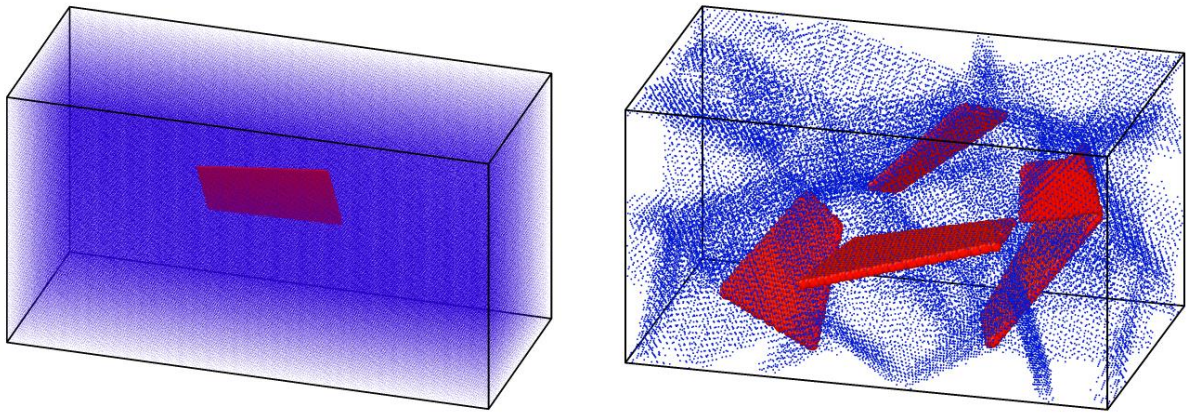
1. Introduction

There exists already a considerable number of experimental and numerical studies on the development of composite materials with carbon modifications (graphite, carbon nanotubes or graphenes) in a metal matrix. For example, in [1,2,3] copper, aluminum, nickel and other metal alloys have been used. Materials either with embedded carbon nanotubes, or graphene exhibit improved properties, such as a strengthening effect, as well as improved electrical and thermal conductivities, etc., but only composites with graphene possess a simultaneous reduction in brittleness [1,2].

2. Simulation of mono- and polycristalline

In the present work, the possibility of improving the mechanical properties of iron by adding dispersed nanoscale graphene discs is examined with molecular dynamics (MD) method. The maximum of shear stresses for sliding edge and screw dislocations with a Burgers vector b = 1/2 [111] moving across graphene sheets with different orientations and sizes of the graphene plate are defined. Also the process of crack formation for various modes of deformation has been considered. The high strength of graphene allows it to serve as an effective barrier to moving dislocations and growing cracks. The molecular dynamics method allows to consider the above processes in a most detailed view.
Due to a shear stress applied in an NVT ensemble of the simulation box, the dislocation starts to move. At the graphene disk the dislocation first comes to a standstill. The applied shear stress is then increased by small increments, until the motion of the dislocation beyond the graphene discs occurs either by cutting or circumvention. In this way, the critical shear stress to overcome the obstacle of the graphene disk can be calculated. These calculations are to be carried out for each of the monocrystals as well as for crystals with different arrangements of graphene discs as obstacle fields. The optimal size, orientation, spatial arrangement and concentration of the graphene discs to achieve a high critical shear stress have been determined. From tensile tests the mechanism of crack propagation in an iron monocrystal was investigated. Graphene as strong barriers resisting crack propagation was thus demonstrated and confirmed from MD simulations.
Strength and the elastic and plastic behavior of a graphene reinforced Fe alloy is examined by applying MD simulations. To achieve this, computer simulations of tensile experiments with suitably selected simulation boxes are performed until breakage of the sample, so the stress-strain curve dependence on size and orientation of graphene slices is obtained. In particular, in these simulations the temporal evolution of lattice defects such as dislocations and possible nanocracks at the Fe-graphene interface is in the center of interest. Simulations for a monocrystal with graphene, see figure 1a or polycrystals with different grain sizes are carried out, see figure 1b.
Fundamental understanding of crack initiation and crack propagation in the system Fe-graphene is expected. The aim of these simulations is to discover similarities and differences of the influence of tensile or pressure loads on the strength properties of Fe-graphene. The main interest in each case is the plastic deformation, the formation and movement of dislocations and the nanocrack

propagation. To achieve this, polycrystals each with a fixed grain size of about 10 nm with differently distributed orientations are created, which due to the lattice mismatch at the grain boundaries contains geometrically necessary dislocations. From this point tensile tests, shear tests and nanoindentation at different temperatures are performed until new dislocations are found. In result of these simulations the mechanisms of the strength increase in the polycrystalline Fe-graphene composite are obtained. Relevant graphene orientations are investigated such as crossing a grain boundary inside a grain, or lying along a grain boundary. As a result, an initial state for the following simulations in the region of high plastic strains are created, hereby the essential foundations for studying the increase in strength properties are performed.



a **b**

Figure 1. (a) Monocrystal and (b) polycrystal containing graphene slices

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