Prof. Dr. rer. nat. Dr. h.c. Siegfried Schmauder, Universität Stuttgart

DFG-Projekt:
MD-Simulation zur Festigkeitserhöhung durch Graphen in Eisenkristallen

In Eisenlegierungen spielt die Erhöhung der Festigkeit durch die Mischkristall-, Teilchen-, und Korngrenzenverfestigung eine herausragende Rolle für die technische Anwendung der Werkstoffe. In diesem Projekt wird der Einfluss von in die Eisenmatrix eingebauten nanoskaligen Graphenscheibchen bzw. von gelöstem Kohlenstoff auf die mechanischen Eigenschaften mit Hilfe von ab-initio- und Molekulardynamik(MD)-Simulationen untersucht. Durch die Zugabe von Graphenscheibchen wird eine Verbesserung mehrerer mechanischer Eigenschaften erwartet. Hierbei sind insbesondere die thermische Stabilität der Graphenscheibchen sowie die Eigenschaften Elastizität, Festigkeit und Plastizität des Eisen/Graphen-Verbundwerkstoffs von Bedeutung.
Zur Abschätzung der thermischen Stabilität der Graphenscheibchen werden ab-initio-Simulationen durchgeführt, die auch für eine Verbesserung der interatomaren Potenziale für die MD-Simulationen verwendet werden.
Danach werden Molekulardynamik-Simulationen jeweils für Ein- und für Polykristalle für unterschiedliche Temperaturen, Kohlenstoff- bzw. Graphenkonzentrationen, Größe sowie Abstände und Orientierungen der Graphenscheibchen durchgeführt. Die Ziele der Berechnungen sind grundlegende Erkenntnisse zu Versetzung/Partikel-Interaktionen, Spannungsfeldern, den durch die legierten Kohlenstoffatome bzw. Graphenscheibchen verursachten Eigenspannungen im Kristallgitter sowie der damit verbundenen Änderung der mechanischen Eigenschaften dieser Materialien.
Hiermit wird erstmalig mittels MD-Simulationen untersucht, ob und inwieweit sich die Eigenschaften von Eisenwerkstoffen durch Zugabe von Graphenscheibchen in die erwünschte Richtung maximale Festigkeit bei maximaler Elastizität bzw. höchstmöglicher plastischer Verformbarkeit (Duktilität und Bruchdehnung) verbessern lassen.

MD simulations of strengthening by graphene in iron crystals

In iron alloys, the increase in strength caused by solid solution, precipitate and grain boundary strengthening, plays an outstanding role in the technical application of the materials. In this project, the influence of nanoscale graphene discs embedded into the iron matrix and of carbon in solid solution on the mechanical properties, respectively, is investigated by means of ab initio and molecular dynamics (MD) simulations. The addition of graphene disks is expected to improve several mechanical properties. In particular, the thermal stability of the graphene discs and the properties of elasticity, strength and plasticity of the iron/graphene composite material are of importance.
To estimate the thermal stability of the graphene discs, ab initio simulations are performed, which are also used to improve the interatomic potentials for the MD simulations. Molecular dynamics simulations using single- and polycrystals will be performed for different temperatures, carbon and graphene concentrations, as well as for different sizes, distances and orientations of the graphene discs.
The objectives of the simulations are fundamental findings concerning dislocation/precipitate interactions, stress fields and residual stresses in the crystal lattice caused by the graphene discs or alloyed carbon atoms, and the associated changes in the mechanical properties of these materials.
For the first time, MD simulations are used to investigate whether and to which extent the properties of iron can be improved by the addition of graphene discs in the desired direction of maximum strength with maximum elasticity and best possible plastic deformability (ductility and fracture strain) respectively.

Results:

Fe{110}/graphene interfaces were relaxed using molecular dynamics simulations using EAM potentials for the Fe interactions [1], AIREBO potentials for the C interactions [2] and Lennard-Jones potentials (ε = 0.043, σ = 2.221) for the Fe-C interactions. The simulations were performed for the structures described in [3,4] where graphene is adsorbed on a Fe{110} surface as well as for the corresponding bulk structures where graphene replaces one Fe{110} monolayer.
Obtained results agree well with ab initio calculations and experimental findings regarding work of separation, averaged normal distances across the interface and corrugation of surface layers.

	W_{sep} [J/m^2] (this work)	W_{sep} [J/m^2] (literature data)	d_{av} [Å] (this work)	d_{av} [Å] (literature data)
Graphene on surface, orientation 1 [3]	0.97	-	2.16	2.32 [3]
Graphene on surface, orientation 2 [4]	0.92	0.89 [4]	2.19	2.11 [4]
Graphene in bulk, orientation 1	0.97	-	2.16	-
Graphene in bulk, orientation 2	0.94	1.0 [4]	2.18	2.3 [4]

Table 1: Work of separation and averaged normal distances of Fe{110}/graphene interfaces.

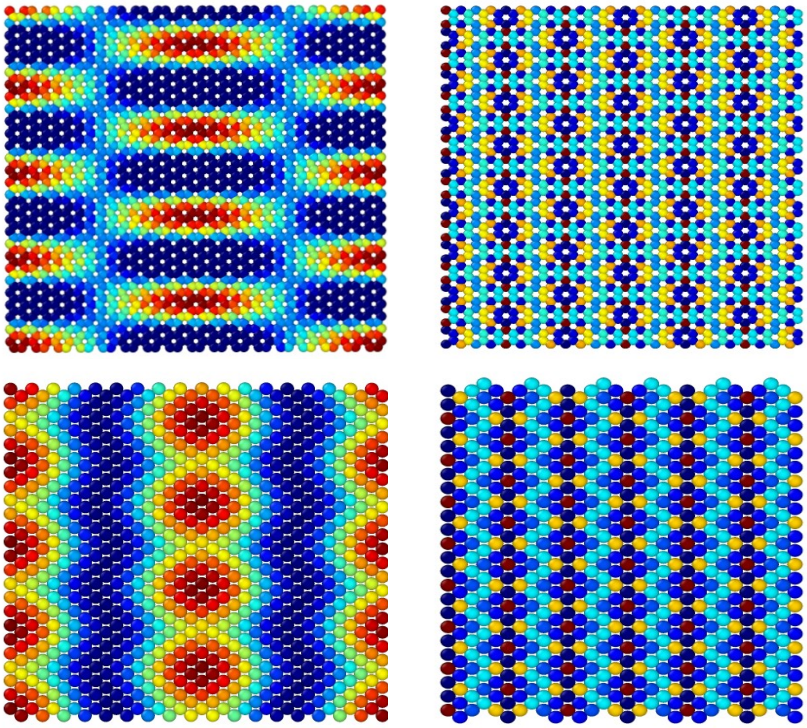

Fig. 1: Atomic coordinates of surface structures (orientation 1: left, orientation 2: right) in direction towards the surface (z). Top: Graphene layer. Bottom: Fe interfacial layer. Colour coding: dark red: high z, dark blue: low z.

As shown in Fig. 1 the graphene layer as well as the Fe interfacial layer of orientation 1 show pronounced regions with high or low atomic coordinates normal to the interface. This buckling leading to a similar corrugation pattern as shown in Fig.1 has been also observed in experiments and ab initio calculations [3]. Furthermore, the results agree regarding the observation that the corrugation of the Fe interfacial layer follows the corrugation of the graphene layer. The simulation results of orientation 2 reveal that the corrugation of graphene and Fe is opposite in this case. Moreover, the graphene atomic coordinates normal to the interface vary in a range of 0.043 Å only whereas a range of 0.32 Å is obtained in case of the strongly buckled surface in orientation 1.

Tensile tests were simulated using the bulk structures where the graphene layer replaces a Fe{110} monolayer. Uniaxial tension was applied in the direction normal to the interface or in directions in the interface plane. In case of tension normal to the interface the tensile strength decreases significantly compared to the corresponding structure of Fe without graphene. The reason is that fracture at the interface occurs already at rather low stresses (Fig. 2, top). In contrast to this behaviour, the tensile strength is higher than in pure Fe in case of tension in directions in the interface plane. It is observed that the graphene layer makes the material stiffer resulting in a stronger increase of the stress strain curve. In this case there is no crack propagation along the interface, instead small pores and dislocations nucleated at the interface are found (Fig. 2, bottom).

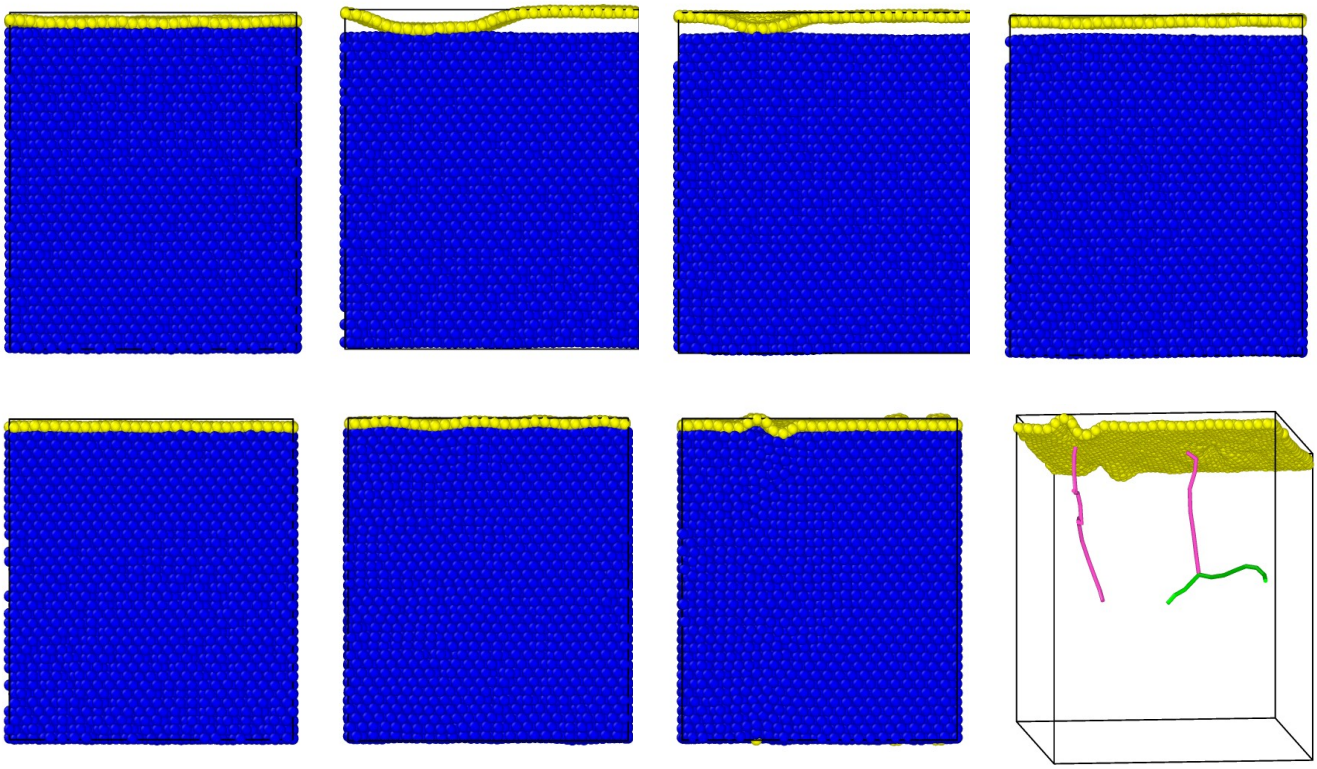

Fig. 2: Material failure during tensile tests with tension normal to the interface (top) or tension along a direction in the interfaces plane (bottom).

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