124th MSS-Seminar
Wednesday, December 12th,
15:30 hrs, Nägelsbachstr. 49b.

Molecular Dynamics Simulations in Materials Sciences: Laser Ablation and Precipitation Strengthening

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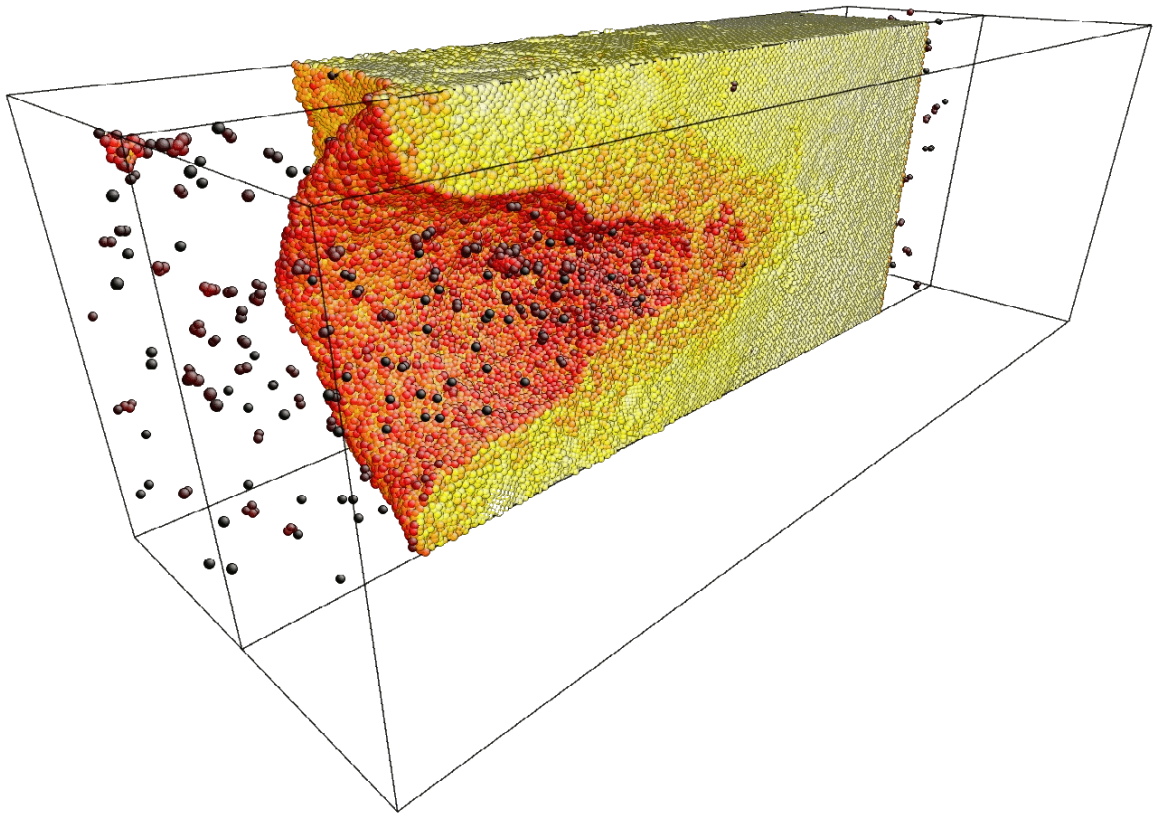

In the first part we will present results from simulations of laser ablation of Al-Ni alloys. Several AlNi intermetallic compounds have then been studied. The general behavior is typical for ablation but both Al_3Ni and $AlNi_3$ show interesting phenomena like phase transitions and dependency of ablation mechanism on fluence. Several different configurations of Al-Ni multilayers have also been simulated. As aluminum has a much lower melting temperature than nickel, the process is dominated by the behavior of nickel. For example we find that it is possible to produce AlNi alloys on aluminum, but not on nickel.

In a second part we will talk about the interaction of NiSi precipitates with dislocations in a copper matrix. Depending on the orientation of the Ni_2Si platelets the precipitate is cut or circumvented. The same happens for spherical Ni_3Si, but there the result also depends on the interaction. If two dislocations meet a precipitate, then the results depends on their relation. The shape of Ag precipitates and their interface with the Cu matrix has been simulated as a function of lattice parameters and the disclocations involved have been determined. Finally, the formation of NiSi precipitates in Cu from solution has been studied. Due to the time scale it is not possible to study this effect with MD which forced us to develop a new combined MD-Monte-Carlo method.