Development Semi-Empirical Potentials Appropriate for Simulation of Mechanical Properties of Metallic Alloys

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Molecular dynamics (MD) simulation of mechanical properties requires reliable but not computationally expensive interatomic potentials. The methods of development of such potentials for metals will be discussed in this talk. A special attention will be paid to the problem of incorporating in the potential development procedure such crystal defect properties as vacancy and interstitial formation energies, staking fault and surface energies. Examples of potentials for fcc, bcc and hcp metals will be considered. Next, the methods of description of interatomic interaction in metallic alloys will be discussed. Cu-Zr amorphous alloys will be used as example to show that the properly developed semi-empirical potentials provide reliable predictions for the concentration and temperature dependence of elastic properties. Finally, the results of MD simulation of plastic deformation in these alloys will be presented. In particular it will be shown that the atomic mobility significantly increases within the flow softening regime.