INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

ICAMS Seminar

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Links between mesoscale and atomistic simulations

Today, computer simulations in materials science have gained a level of maturity where quantitative property predictions can be achieved for real, complex materials. In many cases this requires the simulations to consider a number of physical processes and effects concurrently, in other cases it is essential to bridge wide ranges of time and length scales. In the present talk, cases of links between atomistic and mesoscale simulations are addressed: simulations of the yield stress contributions of (i) precipitates and (ii) solute atoms based on molecular dynamics (MD) and dislocation dynamics, and (iii) MD simulations of grain boundary (GB) mobility to be used in mesoscopic recrystallization or grain growth. In (i) and (ii), an understanding of the relevant mechanisms on the mesoscale is required before relevant quantitative input data can be derived from atomistic simulations. On the other hand for (iii), MD simulations of GB migration in bicrystals indicate that this motion is fundamentally different: Here it seems to be the atomistic mechanisms, differing for each individual GB geometry, that control the velocity. Since several mechanisms are conceivable, in general, and local fluctuations in stresses or strains may chose the active one, it seems impossible at present to derive GB mobility data relevant for mesoscopic polycrystal simulations from MD simulations in bicrystals alone. This link between atomistic and mesoscale simulations appears incomplete.