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ADVANCED MATERIALS SIMULATION

Special Seminar

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Paris, France,

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ICAMS Special Seminar room UHW 11/1102

Different approaches to study alloys using atomistic simulations

During my talk, I will discuss the recent developments of simulation tools we have developed to study properties of materials at atomic scale. First, I will present a tight-binding potential for transition metals, carbon and transition-metal carbides, which has been optimized through a systematic fitting procedure [1]. The Ni-C is more specifically discussed. The successful validation of the potential for different atomic configurations indicates a good transferability of the model and makes it a good choice fo atomistic simulations sampling a large configuration space. By way of example, the catalytic nucleation of carbon nanotubes is discussed using our model coupled to canonical and grand canonical Monte Carlo simulations [2]. The second part will be devoted to the study of Fe-Al alloys which are very promising to meet the industrial demand for high-performance materials. Since a large number of their properties are highly sensitive to the type and concentration of defects present in the material, we have investigated the properties of vacancies (V) and defects to study the stability of VnAlm clusters in the very dilute limit. The approach proposed here combines ab initio (Siesta code), simple thermodynamics and Kinetic Monte Carlo [3].

[1] H. Amara, J.-M. Roussel, C. Bichara, J.-P. Gaspard, and F. Ducastelle, Phys. Rev. B 79 014109 (2009)

[2] H. Amara, C. Bichara, and F. Ducastelle, Phys. Rev. Lett. 100, 056105 (2008)

[3] H. Amara, C. C. Fu, F. Soisson, and P. Maugis, Phys. Rev. B 81, 174101 (2010)