Scientific Report - ESF short visit grant 1982

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Purpose of the visit

The Saclay and the Oxford group are both working on the multi-scale modelling of radiation damage in wall materials for future fusion power plants. It was the purpose of my visit to discuss the methods and simulation techniques used in both groups. In this way possible collaborations that would be mutually beneficial could be discussed.

Description of the work carried out during the visit

During my stay in Paris, I discussed with a number of scientists from CEA Saclay as well as from LEM Onera/CNRS a broad range of modelling problems that are of interest for the activities of the Oxford group. In the following I give only a very brief summary of the topics of the discussions.

- *Hakim Amara*
  development of potentials for the system Fe-C for modelling the growth of single walled carbon nanotubes, simplified models of magnetism, self-consistent Stoner model appears to be too computationally expensive, evaluation of solubility limit using the kinetic Monte Carlo method

- *Manuel Athenes*
  modelling of the six-jump diffusion cycle, analytic solution, Monte Carlo simulations of diffusion

- *Yan le Bouar*
  electron microscopy of small clusters, alloyed nanoparticles, in particular Co-Pt

- *Emmanuel Clouet*
  CVM simulations in Fe-Cr system, kinetic modelling of $Al_3Zr_xSc_{(1-x)}$, diffusion mechanisms

- *Francois Ducastelle*
  angular dependence of interatomic potentials and importance for establishing hierarchy in cluster expansions, concentration dependent cluster expansion coefficients in the CPA and relation to concentration independent coefficients, problems associated with s-d hybridisation in tight-binding model of Ni, modelling of magnetism in Fe-C, modelling of the melting of small clusters

- *Alphonse Finel*
  modelling rafting in superalloys, phase field with inhomogenous elasticity and plasticity, wetting of anti-phase boundaries

- *Mihai-Cosmin Marinica*
  improved parameterization of EAM potentials for Fe by taking into account Peierls barrier, magnetic Dudarev-Derlet potential predicts the wrong core structure, importance of magnetic contribution in Peierls barrier, magnetic tight-binding appears to be not much more efficient than ab-initio calculations using the SIESTA code

- *Maylise Nastar*
  ab-initio calculations for Fe-Cr, contribution of magnetic interactions to the ordering tendencies at low Cr concentrations, diffusion in the Fe-Cr system and kinetic Monte Carlo modelling of diffusion

- *Frederique Soisson*
  Cu precipitation in Fe, simplified cluster expansion, vacancy diffusion mechanism, relevance of hierarchy of Fe and Cu vacancy energy for diffusion of small Cu clusters

- *Lisa Ventelon*
  dislocation structures and interactions in periodic and cluster calculations, core structure in Fe predicted by the Dudarev and Mendelev potential, discrepancies in the Peierls barrier

Description of the main results obtained

The purpose of my vist was to discuss the overlap of the modelling activities of the Saclay and Oxford groups in the view of establishing collaborations in the future. The main result of my stay is that the activities of both groups show considerable overlap such that both groups could benefit from more intense collaborations.

Future collaboration with host institution

My discussions showed that material systems and simulation methods used by the Saclay group and the Oxford group are very similar. Hence, there is a strong motivation for establishing collaborations in the future.

Projected publications/articles resulting or to result from your grant

I do not think that publications will result from my stay in Paris. I expect that future collaborative projects may lead to joint publications.