

Report on Computer Simulation and Atomistic modelling of Materials

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Introduction

This meeting, organised by the atomic collisions in solids group of the IOP, was attended by 37 participants from various academic backgrounds and industry. An abstract booklet is appended which includes a list of all the invited and contributed talks.

The theme of the meeting was to be both educational and state of the art. The day's programme included discussion of ab-initio potential calculations, semi-empirical potential development, Monte-Carlo and molecular dynamics (MD) simulations and their application to a number of interesting chemical and physical phenomena including novel ionic materials and scanning tunnelling microscopy. The attached abstracts give more detail of the individual lecture content.

An important message which the meeting communicated (besides the rapid development of parallel computing) was the importance of visual representation. All the lectures were elucidated by the use of graphics visualisation packages and during the meeting three MD video presentations were also given. Video presentations are becoming a popular source of disseminating material and the dynamic visualisation of a number of processes revealed features which would have been more difficult to understand and explain without them. The videos showed the process of adhesion and wear of STM tips on a metal substrate, the process of sputtering, implantation and the formation of surface waves by C_{60} molecules on graphite. A final video depicted the process of radiation damage formation in metals by energetic collision cascades.

The general feeling of participants at the end of the meeting was that it had been a useful exercise and one that might well be worth repeating in about 18 months or 2 years time.