UNIVERSITY OF CAMBRIDGE

Master of Philosophy Course
Modelling of Materials

The hierarchy of computer models in materials research; the importance of linking scales.

M. J. Peet

Abstract

Computer models for materials can be made more sophisticated by passing information between different length scales. This article is intended to review the methods for passing information between scales, both sequential and concurrent multiscale techniques are considered.

1. Introduction

The idea of scale has always been a fundamental part in the understanding of materials and materials properties. Figure 1 shows the spatial and temporal scales that are most important to our understanding of materials; the electronic level, atomistic level, microstructural level and the continuum level[1].

The nature of the interactions between different scales of phenomena in complex systems has recently been receiving increased interest from a number of scientific fields.[2, 3] In materials science the challenge is to integrate the various scales to give a holistic picture of the materials.

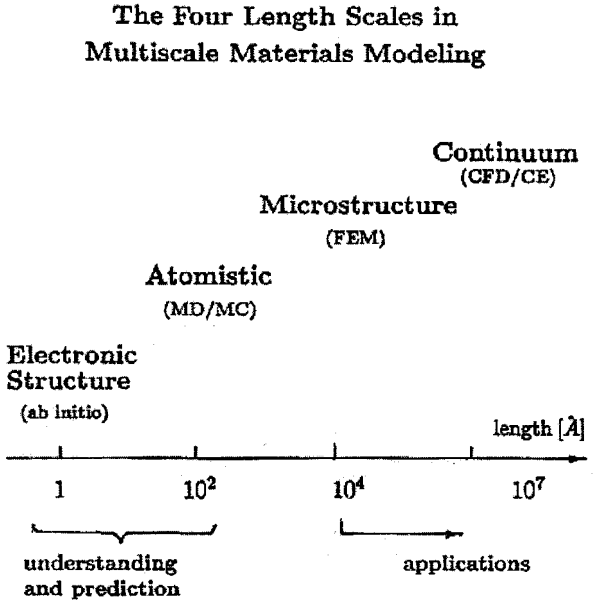

Figure 1, Length Scales in Materials Modelling, S Yid.

Modelling techniques have been developed to model or simulate materials at each length scale, the table below shows the physically relevant scaling parameters in the various models used in computational materials science. The range of scale covered by a particular model is relevant to the reliability of a model since they rely on adequate discretisation of space and time.[4]

Existing hierarchy of computer models[4]

Length Scale (m)	Physical Origin (Upper bound)	Physical Origin (Lower bound)	Simulation Method
10^{0}-10^{-3}	External Load	Cross section reduction, critical reductions	Finite elements, finite difference
10^{0}-10^{-7}	External load	Grain size, dislocation cell size, crack size, particle size	Advanced microstructure finite element models (microstructure mechanics)
10^{0}-10^{-7}	External load	Grain shape	Taylor-Bishop-Hill models
10^{0}-10^{-8}	External load	Grain shape, inclusion shape, cell size	Self consistent models
10^{0}-10^{-9}	System size	Atom	Percolation models
10^{0}-10^{-9}	System size	Atomic clusters	Cellular automata (deterministic of probabilistic)
10^{-3}-10^{-7}	Grain clusters	Dislocation cell size, microband	Boundary dynamics, topological network models, vertex models
10^{-4}-10^{-9}	Grain clusters	Burgers vector, annihilation spacing	Dislocation dynamics
10^{-5}-10^{-9}	Grain clusters	Atom clusters	Continuum field kinetic theory
10^{-5}-10^{-9}	Grain clusters	Structural interface unit, atom clusters	Potts model
10^{-5}-10^{-9}	Grain	Burgers vector, annihilation spacing	Dislocation segment dynamics
10^{-6}-10^{-9}	Grain	Atom clusters	Microscopic field kinetic theory
10^{-7}-10^{-10}	System size	Atom clusters	Cluster variation method
10^{-7}-10^{-10}	System size	Atom clusters	Molecular field approximation
10^{-7}-10^{-10}	System size	Atom	Metropolis Monte Carlo
10^{-6}-10^{-10}	Cell size	Atom	Molecular dynamics (pair potentials, embedded atom potentials)
10^{-8}-10^{-12}	Atom clusters	Ion, electron	Ab initio molecular dynamics (tight binding potentials, local density functional theory)

Computer models of materials are intended to provide a convenient way of predicting and optimising material properties, the various models are increasingly complemented by the idea of integrated modelling and simulation.[5] This linking of several different scale models has become increasingly been encompassed in the concept of multiscale modelling. Multiscale models address the issues pertaining to the different scales and the inter-relations between the scales, before we discuss Multiscale models to link the scales in materials research, it will be useful to discuss the types of models and the importance of linking scales in some more detail. [6]

2. The importance of linking scales

The atomistic simulation of properties and phenomena in solid materials requires a suitable model of the real system, the typical solid contains in the order of 10^{23} atoms, and only a small fraction can be treated explicitly. The effect of the rest needs to be taken account of somehow.[7]

Methods for computing the properties of materials can be divided into two separate approaches; those that use empirically or experimentally derived data, and those that do not. The semi-empirical methods excel at interpolating and extrapolating from known properties. The methods that do not use empirical data are often called ab initio or first principles methods.

Ab initio methods are based on the density functional theory, developed by Kohn, Hohenburg and Sham[8]. The exact solution of the full, many body Schrodinger equation for a system is impossible, but accurate approximations of a systems ground state can be made, such approximations are widely used in condensed matter physics. This method has excellent predictive power when experimental data is scarce or unavilable.[8] Simulations in materials physics aim at predicting microstructural phenomenon using ab-initio molecular dynamics and Monte Carlo methods.

Semi-empirical methods operate beyond the current scale of first principle calculations. For many practical design calculations, either continuum or finite element techniques are most useful. These methods need to be supplied with data about the properties, either from empirically derived results or from calculations done at the molecular and electronic levels. Simulations in materials science pertaining to mechanical engineering typically focus on large-scale construction problems using finite element approaches where the microstructure has been reduced by the incorporation of averaging constitutive laws.

The original domain of materials science could be said to be the investigation of lattice defect ensembles at the mesoscale. The use of simulations in this particular field must bridge enormous space and time scales and provide concepts to describe complex many body interaction phenomena. In contrast to atomistic scale molecular dynamics and Monte Carlo simulations, most mesoscale approaches are formulated as continuum models, often with discrete consideration of lattice defects. These methods include deterministic and probabilistic cellular automata, which may account for both short range and long-range interactions. Examples are Grinzberg-Landau, Cahn-Hilliard, and Allen-Cahn type phase field methods, dislocation dynamics, ploy-crystal and non-linear plasticity finite element models, topological network and vertex models, boundary dynamics, metropolis MC and conventional FE simulations.[4]

The use of computer simulation or numerical methods is promoted by the increasing capability of computer systems in terms of speed and information storage, and by the growing demands for quantitative predictions in industry and research. By including more scales into a model, more of the known materials theory is included, models become more predictive and further understanding can be developed. A holistic model would include interactions at all time and length scales and would allow true predictive modelling of complex structures at the continuum scale where properties such as mechanical properties emerge. [1]

3. Multiscale Modelling Techniques

There are two main approaches to multiscale modelling, one method is the development of hybrid models that bridge different time and length scales, the other are to pass selected information between different models. These two approaches are often referred to as handshaking and handing-off, respectively (Rudd).

In "From Molecular Dynamics To Kinetic Rate Theory: A Simple Example Of Multiscale Modelling" [9] R. E. Stoller and L. R. Greenwood have used the handing-off method using molecular dynamics data to model radiation damage, this is also the approach in the example of crack propagation in silicon.

Since the evolution of microstructure is path dependant concepts of integrated modelling and simulation should therefore include as many of the microstructurally relevant processing parameters as possible. However such a procedure requires the incorporation of various time scales, which can differ by some orders of magnitude. One reasonable approach for combining various scales consists in the incorporation of constitutive laws that have been derived from non-averaged, i.e. space-& time discretised, simulations on the appropriate smaller scale. In such a concept the results from a certain scale are averaged and condensed before being considered at the next scale this means that the phenomelogical character of the model equations used in each step increases with scale.

There have been many conferences and workshops on multiscale modelling these often focus on a sequential approach with individual research groups often focusing on modelling one particular scale with reference to what the input and output parameters are. In multiscale modelling from the first principles to the continuum scale, the biggest challenge is in modelling microstructures. The evaluation of microstructure depends upon the defect thermodynamics and kinetics.

3.1 Examples of linking scales

A multiscale model by Clementi et al in the 1980s linked electronic scale calculations to macroscale phenomena, using sequential coupling.[10] There work used quantum-mechanical calculations to evaluate the interactions of several water molecules, which was used to paramatise an empirical potential for use in molecular dynamics. A molecular dynamics simulatuion was then used to calculate the viscosity of water. The computed viscosity was then used to calculate tidal circulation patterns.

Several good examples of multiscale modelling of crack propagation, implemented using different techniques exist. The first discussed here is by F. Abraham et al and

links the electronic, atomistic and continuum scales to model brittle fracture in silicon, the second is H Rafii-Tabar et al and links the atomistic and continuum scales to study crack propagation in silver.

F. Abraham et al have coupled length scales to model the fracture of silicon as they propose the model as an example of how to solve a multiscale problem using parallel calculations at different scales.[11] For simplicity the example deals with the brittle (ideal) fracture of silicon (ideal solid) under uniaxial tension, but the methods are designed to be generally applicable. The traditional approach to model fracture would be continuum mechanics, but failure mechanisms are not naturally described by this method. At a finer level of classically interacting atoms, material decohesion does arise naturally. Treating bond breaking with an empirical potential may be unrealistic, and a quantum mechanical treatment should give more reliable results. In the case where the crack is moving the three levels need to be brought together to operate seamlessly together. The implementation is achieved using two so-called hand-shaking regions, at the interfaces of the models. The finite element – molecular dynamics (FE-MD) 'handshaking' region and the molecular dynamics – tight binding (MD-TB) 'handshaking' region. The table below summarises the size of each of the three modelling regions.[11]

Table 2, Summary of region sizes, and computational expense

Region	Resolution	Technique	Time Step (s)
FE	258048 mesh points	1 processor	0.7
MD	1,032,192 atoms	24 processors for 24 spatial regions	1.8
TB	280 unique atoms	Eight overlapping regions	1.5

The method of integration is to define a Hamiltonian for the whole system; this will result in a conserved total energy for the system. Equations of motion for relevant variables are taken from appropriate derivatives of the Hamiltonian. The variables can then be updated in lockstep as a function of time using the same integrator.[11]

$$H_{Tot} = H_{FE}(\{\mathbf{u}, \dot{\mathbf{u}}\}\varepsilon\ FE) + H_{FE/MD}(\{\mathbf{u}, \dot{\mathbf{u}}, \mathbf{r}, \dot{\mathbf{r}}\}\varepsilon\ FE/MD) + H_{MD}(\{\mathbf{r}, \dot{\mathbf{r}}\}\varepsilon\ MD) + H_{MD/TB}(\{\mathbf{r}, \dot{\mathbf{r}}\}\varepsilon\ MD/TB) + H_{TB}(\{\mathbf{r}, \dot{\mathbf{r}}\}\varepsilon\ TB)$$

Where degrees of freedom are displacements, $\mathbf{u}$, and rate of change of displacement $\dot{\mathbf{u}}$, and atomic positions $\mathbf{r}$ and their velocities $\dot{\mathbf{r}}$.

In the FE-MD region the FE mesh spacing is scaled to atomic dimensions. The MD model is then embedded into this continuum model. The interactions are taken as the mean of the FE Hookian description and the MD inter-atomic potential description. The FE/MD interface is taken to be far from fracture region so that Atoms and displacements from the FE region can unambiguously be assigned to one another.[11]

For the MD/TB handshake interface, each dangling bond at the edge of the TB region is terminated using pseudo-hydrogen.[11] Although the method is not fully described and Abraham refers the reader to work yet to be published when the article was written.

Unlike the FE-MD handshaking the MD/TB handshaking has to be accomplished across an interface, since computing individual bond strengths is difficult in a computationally efficient way. The MD-TB handshaking takes place across an interface consisting of atoms. The forces in the cluster depend on the position of the silogen atoms so they lead to handshaking between the MD and TB regions.[12]

Since the crack opening is a dynamic process the TB region relocated after every ten time-steps, around the atom nearest the centre of the crack with the highest strain energy.

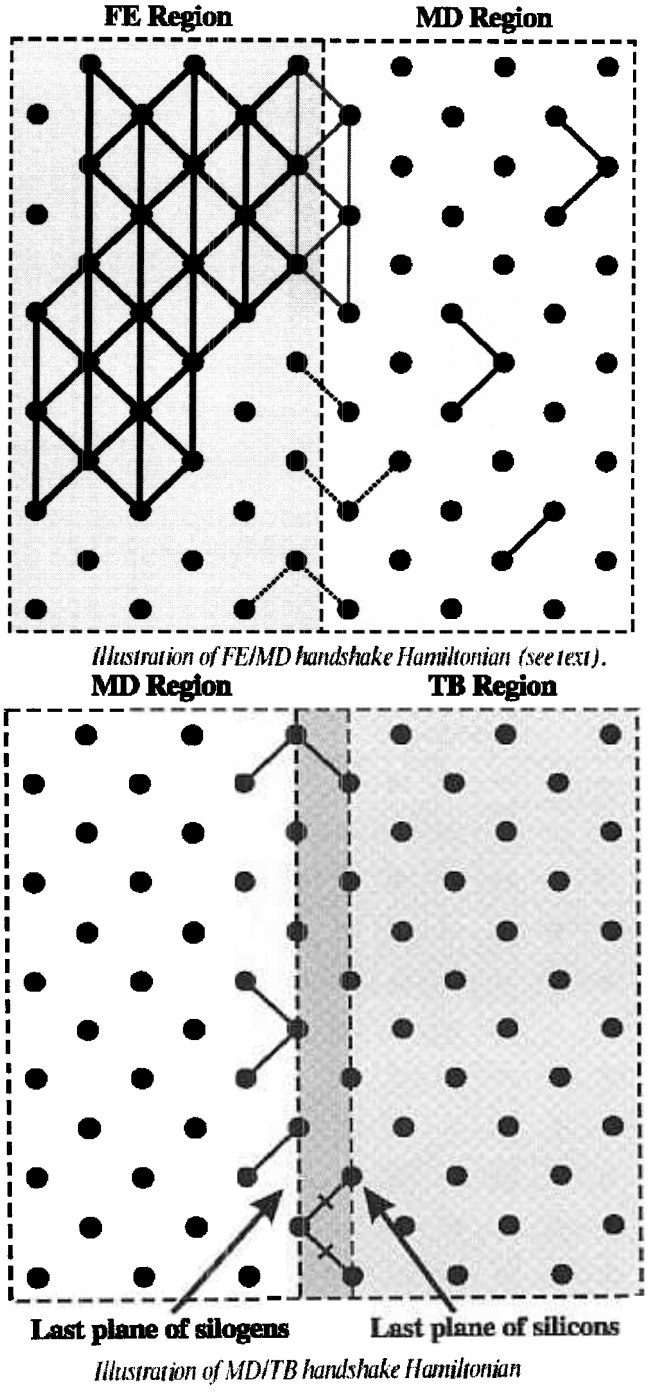

Figure 2, Handshaking regions in multiscale MAAD Silicon model

H Rafii-Tabar et al,[13] have used a different approach to modelling crack propagation, a multi-scale atomistic-continuum model of crack propagation in a two-dimensional macroscopic plate. A seamless multi-scale model is applied to the propagation of a crack. The model couples crack dynamics of the macroscale and nanoscale via an intermediate mesoscale continuum. The methodology is as follows, finite element method is employed to make the transition from the macroscale to the nanoscale by calculating the displacements of the atoms at the boundary of an atomic lattice embedded within the plate and surrounding the crack tip. MD simulation is then used to drive the tip forward, producing the tip critical velocity and the tips diffusion constant in space. These are then used to calculate the Ito stochastic calculus to make the reverse transition from the nanoscale back to the macroscale. The model successfully produced crack velocity oscillations, roughening transitions of the crack surfaces and macroscopic crack trajectory.

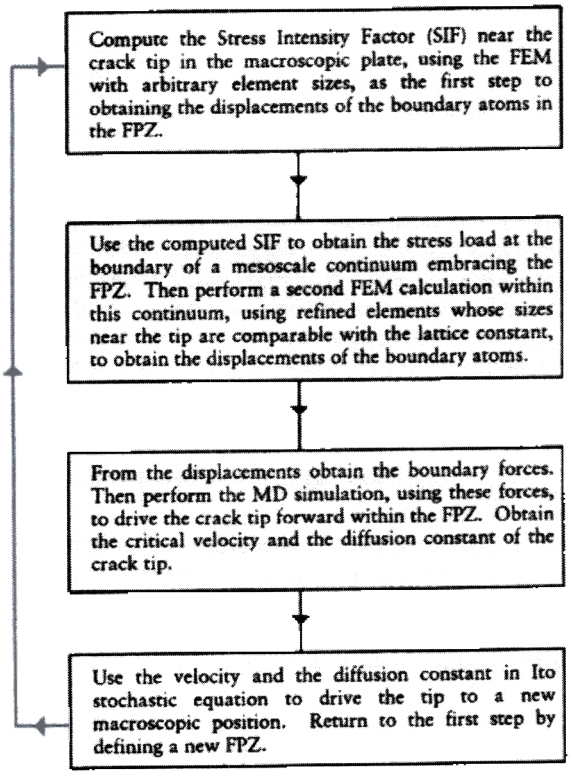

Figure 3, Flow chart summarizing main tasks in atomistic-continuum model for crack growth

R. E. Rudd et al [12, 14, 15] have extended the model used by Abraham et al, for modelling of Micro-Electro-Mechanical systems (MEMS). The design of MEMS hinges on a through understanding of the mechanics of the device, these devices are not large enough to obey the laws of continuum mechanics. The behaviour of the material is decided at an atomistic level rather than a continuum level. The role of surfaces become more pronounced, new mechanisms for dissipation become evident, anharmonic effects become more important, the devices become less stiff than predicted by finite element, statistical mechanics become a key issue. [12] R. E. Rudd et al, argue that for successful handshaking there are several finite size effects that need to be considered, and that particular attention need to be given to the effect of this

non-physical boundary. Attention must be given to Slowly varying strain fields, Thermodynamics, Elastic waves and Non-equilibrium thermodynamics.
A coarse-grained molecular dynamics model is incorporated into the multiscale model, to aid the coupling between the atomistic and finite element regions. Finite element does not connect perfectly smoothly with atomistic when the mesh size is of atomic scale. This can cause problems in some simulations, the cause grained molecular dynamics approach is proposed as a technique to overcome this by replacing the finite element using a similar implementation to the finite element.

The 1997 Workshop on multi-scale modelling had the objectives of; (1) establishing a model system that is well suited to the multi-scale modelling methodology; (2) explore a set of discrete simulation methods at the continuum-scale, meso-scale, micro-scale, and atomic scale; and (3) identify critical links connecting the length scales which allow critical information to be passed among scales and allow the end goal of predictive models at the continuum scale. [15] The workshop considered plasticity as an example of a system well suited to a multi scale approach. The scales of microstructure can be determined with a method of linking the atomistic and mesoscopic length scales known as three dimensional dislocation dynamics. The conclusion reached in the workshop report stated that simple metal plasticity could be addressed at all relevant length scales but that the challenge of passing information between the scales still remained.

There are relatively few examples of the development of hybrid models in the literature there are many examples of passing information between models. The handing-off method is usually used to increase the range of scales that can be modelled, passing information from a smaller scale to a larger scale.

M. A. Miodownik et al, have approached the modelling of recrystallisation with a multiscale technique.[18] the model links a dislocation model, a cell growth model and a macroscopic model. The model is demonstrated by forming a realistic microstructure using information from the dislocation model. The dislocation model is employed to examine the dynamics of dislocation boundary motion. This information is passed into a mesoscopic simulation which models cell boundaries, allowing the simulation of a large number of cells. Parameters such as nucleation rates and nuclei orientation are fed from the mesoscopic model into a macroscopic model of recrystallisation.

R. E. Stoller and L. R. Greenwood combined molecular dynamics simulation results with kinetic models for radiation damage to provide a better estimate of service life in nuclear reactors.[9] Molecular dynamics has seen extensive application in simulating displacement cascades and advances in computing have allowed greater numbers of atoms to be simulated and hence higher energy events can be examined. The results from the molecular dynamic simulations provided an improved primary radiation damage source term in kinetic models. The kinetic models are typically the solution of simultaneous equations to predict swelling, irradiation creep, or embrittlement. The model was used to investigate temperature and radiation energy effects.

Other examples of multiscale modelling research include; integrated systems design of advanced steels, dislocation dynamics in bcc transition metals, and the investigation of hydrolytic weakening in quartz.[1]

Dislocation dynamics in bcc transition metals at the Lawrence Livermore Laboratory with a multiscale approach to generating constitutive relations for high strain rate deformations in bcc transition metals. Hydrolytic weakening in quartz – this problem involves understanding the loss of compressive strength in hydrated SiO_2. A major challenge is to understand the effect of water bonding at a crack tip. Electronic structure calculations coupled to atomistic and mesoscale simulations are required to bring about a realistic treatment of how chemical reactivity affects mechanical behaviour.

4. Conclusions

A range of models have been discussed which have demonstrated various ways of passing information between the different scales. While some of the terminology is new many of the ideas are intuitive especially where the modelling is done sequentially. Hybrid models that model several scales in parallel are a recent development and there has been some discussion of the methods. It is believed that this approach will have great significance to materials research in the future; the current challenge is to integrate the different scales.

5. References

1. S. Yipp, *Molecular Dynamics Simulation for Materials Processing*, Notes for a short intensive course. July 2000.
2. Workshop on Multiscale Phenomena, Modelling and Computation, Eliat March 2-7 1997.
3. E. Clementi, *Global scientific and engineering simulations on scalar, vector and parallel LCAP-type supercomputers*, Philos. Trans. R. Soc. A 326, 445-470 1988.
4. Dierk Raabe, *Computational Materials Science: The Simulation of Materials, Microstructures and Properties*, Weinheim; Chichester: Wiley-VCH, 1998.
5. G. Gottenstein, D. Raabe, *Integral modeling of metallic materials*, Current Opinion in Solid State Physics & Materials Science, 3 1998, pp244-268
6. N. Ramakrishnan and P Ramarao, *Computer modelling and simulation in materials science*, Bulletin of Materials Science, Vol 22, No. 5, August 1999.
7. P. Deak, *Choosing Models for Solids*, Phy. Stat. Sol. (b) 217, 9, 2000.
8. J. Bernholc, *Computational Materials Science: The Era of Applied Quantum Mechanics*, Physics Today, September 1999, pp30-35.
9. R. E. Stoller and L. R. Greenwood, *from molecular dynamics to kinetic rate theory: A simple example of multiscale modelling*, Proceedings of MRS 1998 Fall Meeting, Symposium J: Multiscale Modelling of Materials. (As-revised 11 Jan 1999).
10. E. Clementi, *Global scientific and engineering simulations on scalar, vector and parallel LCAP-type supercomputers*, Philos. Trans. R. Soc. A 326, 445-470 1988.
11. F. F. Abraham et al, *Spanning the length scales in dynamic simulation*, Computers in Physics, Vol. 12, No. 6, Nov/Dec 1998.
12. R. E. Rudd and J. Q. Broughton, *Atomistic simulation Of MEMS resonators through the coupling of length scales*, Journal of Modeling And Simulation of Microsystems, Vol. 1, No. 1, Pages 29-38, 1999.

13. H. Rafir-Tabar, L. Hua and M. Cross, *A multi-scale Atomistic-Continuum modelling of crack propagation in a two-dimensional macroscopic plate*, Journal of Physics of Condensed Matter, v10, n11, 1998, pp2375-2387.
14. R. E. Rudd and J. Q. Broughton, *Concurrent coupling of length scales in solid state systems,* Phy. Stat. Sol. (b) 217, 251, 2000.
15. R. E. Rudd and J. Q. Broughton, *Coupling of length scales and simulation of MEMS resonators*, Condensed Matter, 14 Dec 1998.
16. G. H. Cambell et al, *Multi-scale modeling of polycrystal plasticity: a workshop report*, Materials Science and Engineering A, 254, 1998, pp 1-22.
17. Y. Estrin, *Syntheses: Playing scales – a brief summary,* Model. Simul. Mater. Sc. 7(5) 747-751 Sep 1999
18. M. A. Miodownik et al, *Multiscale modelling of recrystallization,* Materials research society, Proceedings of MRS 1998 Fall Meeting, Symposium J: Multiscale Modelling of Materials, 1999, p157-162