Chapter 15.

Dislocation-dynamics method

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Abstract

Dislocation-Dynamics (DD) technique is identified as the method able to model the evolution of material plastic properties as a function of the microstructural transformation predicted at the atomic scale. Indeed, it is the only simulation method capable of taking into account the collective behaviour of a large number of dislocations inside a realistic microstructure.

DD simulations are based on the elastic dislocation theory following rules inherent to the dislocation core structure often call "local rules". All the data necessary to establish the local rules for DD have to come directly from experiment or alternatively from simulations carried out at the atomic scale such as molecular dynamics or *ab initio* calculations. However, no precise information on the interaction between two dislocations or between dislocations and defects induced by irradiation are available for nuclear fuels. Therefore, in this article the DD technique will be presented and some examples are given of what can be achieved with it.

Introduction

Usually plastic deformation of single crystals is carried out by large number of dislocations. Dislocation theory enhanced by experimental tools such as Transmission Electron Microscopy (TEM) has made significant advancements in understanding the plastic behaviour of crystalline materials. However, due to the multiplicity and complexity of the dislocation mechanisms involved, there exists a huge gap between the properties of individual dislocations and unit dislocation mechanisms at the microscopic scale and the material behaviour at the macroscopic scale. To translate the fundamental understanding of dislocation mechanisms into a quantitative physical theory for crystal plasticity, a new means of tracking the dislocation motion and interaction over large time and space evolution

is needed. In a multi-scale approach, three-dimensional Dislocation-Dynamics (DD) simulation is the only link between the atomic and the continuum aspects of plastic deformation. At the atomic scale, simulation methods such as *ab initio* or molecular dynamics allow studying very local phenomenon such as the structure of dislocation core, and the interactions between a dislocation with other point defects, dislocations or impurity. These simulations calculate directly the interactions between atoms in the crystal. Therefore, they are limited on the number of atoms that can be simulated because, in 3D, those numbers increase by the cube of the system size. They can only model small volumes ($< 10^{-6}$ μm^3) for very small amount of time ($<10^{-9}$ s). On the other hand, at the macroscopic scale, plastic deformation is generally treated in continuum mechanics through phenomenological laws.

In this article, we will describe the method. According to our knowledge, no DD simulation has been done in nuclear fuels, all the citations related to DD studies refer mainly to metals.

Dislocation-dynamics method

DD simulations are dedicated to the study of the plasticity mechanisms through the collective behaviour of a large number of dislocations. In DD, the discrete nature of the crystalline lattice is not explicitly described, hence the volume that can be simulated with this technique reaches 10^3 μm^3 typically. This length scale is sufficient to represent the plastic deformation at the mesoscale level and to take into account the complex phenomena due to the collective properties of dislocations. It produces stress-strain curves and other mechanical properties, and allows detailed analysis of the dislocation microstructure evolution.

The basic idea of DD simulations is to compute the motion of each dislocation based on a spatial and time discretisation. The dislocation line is represented by connected discrete line segments. An effective driving force is computed for every segment according to the dislocation line tension, dislocation interaction forces and external loading. The dislocation segments respond to these forces by making discrete movement according to a mobility function that is characteristic of the dislocation type and the specific material being simulated. The dislocation mobility can be extracted from experimental data, or calculated by atomistic simulations. And the mobility is one of the key inputs to a DD simulation. Another important consideration for DD simulations is dealing with close dislocation-dislocation interactions such as annihilation and junction formation and breaking. These close interactions can be very complex and usually require special treatment. An efficient way to deal with them is to use prescribed "rules". A bottleneck for DD simulation is the calculation of the elastic interactions between dislocations which is long range in nature. In order to perform DD simulations for realistic material plastic behaviour, efficient algorithms must be developed to enable the simulation over reasonable time and space range with a large number of dislocations.

Historically, the first DD codes, which describe the collective properties of dislocations appeared at the end of the 1980s [19,12]. These bi-dimensional simulations have shown some microstructure formation during plastic deformation with a parallel infinite dislocation lines. However, these simple two-dimensinal codes are limited and do not take into account some important dislocation properties such as: dislocation

multiplication mechanisms, line tension effects or dislocation junction formation. Recently, original works have been published in order to improve these simulations [1,14]. The first tri-dimensional DD code appeared at the beginning of the 1990s [17] and demonstrated that the limitations encountered with the first simulations disappear with three-dimensional approach. Today, several three-dimensional models exist [6,16,9,13,27,34,7,32,3] and the strength and drawbacks of each model are still subject to debate [28,20,2]. Alternatively, other approaches to study dislocation properties at the mesoscale exist [8,31,33]. However, they remain marginal compared to DD simulations for which the number of users increases continuously.

Although most of the DD simulations carried out are under uniaxial load, the physical problems treated are varied. Among the problems already issued we can list for instance:

- forest hardening [5,21,24];
- nanoindentation [10];
- scaling effects [26,18];
- dislocation clustering [21];
- fatigue [25];
- temperature and strain rate effects [29,22].

Conclusions and future challenges

DD simulation is the link between atomistic scale simulations that describe the discrete local physical phenomena and the macroscopic scale that is treated with mechanics continuum method. This method gives the behaviour of the plastic deformation, which is mainly due to dislocation motion and clustering. Up to now, no DD simulation has been carried out in nuclear fuels. This is partly due to the fact that some key input parameters necessary to run DD simulations such as: dislocation mobility and dislocation interaction are missing or are not yet well described. This information is uneasy to obtain experimentally because dislocations appear mainly in nuclear fuels under irradiation. An alternative would be to conduct atomistic calculations to estimate these data. Recently, there has been a renewed interest in dislocation modelling in UO_2 exclusively with molecular dynamics simulations: [23,4,11,15]. However, these studies are still incomplete. For instance, some DFT calculations confirming the glide planes and the Peierls barriers would be useful. More investigations on the dislocation interaction forces would also be valuable. Nevertheless, with some assumptions, some DD simulations could be performed with success.

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