Progress and challenges in finite element simulation of nanoindentation of ion-irradiated materials

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Abstract: In recent decades, nanoindentation technology has been recognized as an effective method to test the mechanical properties of materials at the micro-nano scale. It is widely used in various fields of material science and is currently used in the testing of mechanical properties of ion-irradiated materials. New phenomenon and problems by the combination of nanoindentation technology and ion irradiation have been discovered. The finite element method is a numerical simulation method suitable for simulating this physical process. Using finite element simulation, we can develop a deeper understanding of the physical process. This article reviews some studies on the measurement of the mechanical properties of ion-irradiated materials with nanoindentation technology and their simulations, summarizes the characteristics of the current theoretical model, and discusses the key physical problems encountered in the simulation process and current solutions in order to support further analysis of the nanoindentation mechanism of ion-irradiated materials.

1. Introduction
With abundant reserves, high energy density and low carbon, nuclear energy is a promising way to meet the huge energy demand. Ion irradiation techniques has its unique capability in the research and development of advanced irradiation resistant structural materials. Compared with neutron irradiation, ion irradiation has a shorter experimental period (the dose rate of ion irradiation is 3-7 orders of magnitude higher than that of in-pile irradiation), much lower cost, more abundant irradiation source and lower radioactive intensity of irradiated samples etc., therefore it is widely used in the study of irradiation behaviors^{1,2}. However, the penetration range of ion irradiation is very short, usually only a few microns to tens of microns. Since the 1990s, with the intensive research on the mechanical properties of micro-nano-scale materials, nanoindentation technology has been developed and evolved rapidly. The advantage of nanoindentation is that it can measure mechanical properties such as hardness, elastic modulus, and yield strength in small-scale, and is suitable for thin film samples or superficial layers of the samples. However, the nanoindentation technology itself has some unresolved problems. The indentation process introduces complex compressive and tensile stresses, and the plastic zone results in the indentation size effect (ISE) and other problems. The plastic zone radius is usually several times of indentation depth. Nanoindentation measures not only the mechanical properties of a certain indentation depth of the material, but also the inhomogeneous distribution of defects depending on depth caused by ion irradiation. The coupling of the two makes the problem even more complicated. The nanoindentation measurement and research of ion-irradiated materials has brought many difficulties, and challenges in the data analysis and interpretation of micro-mechanisms.

The indentation is a complex mechanical process. The microscopic deformation of the material under the indenter is not only related to the properties of the material itself, but also related to the
properties and geometry of the indenter, and even to the loading mode of the indentation. It is difficult to obtain the full field analytical solution. The numerical simulation provides a new direction for studying such mechanical problems. Through numerical simulation, not only can the whole physical process be visualized and intuitive, but it also facilitates the research under different experimental conditions, and helps to understand the micro mechanism in the indentation process. Among the numerical simulation methods, the finite element method is the most widely-used tool for studying the nanoindentation on the time and space scale.

The arrangement of this paper is as follows. In the second section, typical problems encountered in the study of the finite element method of nanoindentation are introduced, which lead to the crystal plasticity theory. The third section introduces the crystal plasticity finite element method (CPFEM) used to study the micro-nano scale problem. In the fourth section, for the unique problems of ion-irradiated materials, some current simulation researches are highlighted. A short summary is given in the last section.

2. Typical problems of finite element simulation of nanoindentation

Finite element simulation can help extracting the mechanical properties from nanoindentation tests. The various stress-strain relationship can be obtained from the FE simulations using presumed material properties and loading-unloading scheme with different settings. The extraction procedure is as follows: First, establish the dimensionless function relationship between the shape parameters of the load-displacement curve and the parameters of the material stress-strain relationship using the dimensional analysis method. The second step is to set the mechanical parameters of some materials and simulate the load-displacement curve through the finite element method to verify the correctness of the dimensionless function. Finally, input the load-displacement data obtained from the nanoindentation test, and inversely deduce the stress-strain relationship based on the dimensionless function. For bulk materials, this idea is successful, but for thin film materials, this method has encountered difficulties. This mainly comes from the peculiar substrate effect and ISE of the film material. If the indentation is too deep, the substrate effect is obvious, and if the indentation is too shallow, the size effect is obvious.

During the nanoindentation process, the material undergoes elastoplastic deformation, and a plastic zone that exceeds the indentation depth appears. The stress in the plastic zone affects the load-displacement curve of indentation. For the nanoindentation of the film, if the plastic zone exceeds the depth of the film, the result will be disturbed by the substrate and not entirely the properties of the film. Studies have shown that when the indentation depth is within one-tenth of the film thickness, the influence of the substrate effect can be eliminated. If the plastic zone exceeds the thickness of thin films, notable substrate effect can exist and must be taken in consideration in experimental data analyzes.

When the indentation depth is less than 1 micron, the ISE appears, and the measured hardness increases as the indentation depth decreases. External factors such as work hardening, oxidation, contamination, roughness of the sample surface may also contribute. However, the size effect still exists after excluding these external factors.

The most famous physical model explaining the size effect of indentation is the strain gradient plasticity theory of Nix and Gao. When the material is under stress, the micro-structure forms a plastic deformation gradient, and dislocations are stored in it to adapt to the deformation gradient. This kind of dislocations that enable various parts of the material to be deformed compatible is called geometrically necessary dislocations (GNDs) to distinguish them from the statistically stored dislocations (SSDs) accumulated by capturing each other in a random manner. The array of GNDs hinders the movement of the mobile dislocations, which manifests as work hardening in the macroscopic view. During the nanoindentation process, under the action of the indenter, a plastic zone with dislocation nucleation will appear in the indentation area. The size effect is caused by the change of the GND density induced by the strain gradient.
Based on the dislocation model of Nix and Gao, Gao and Huang\cite{9,10} proposed a strain gradient plasticity theory based on the dislocation mechanism, which has been able to explain the size effect of the indentation process well.

The theory of the traditional finite element method is based on the classical plasticity theory of continuum. It does not include any scale factor related to material properties, that is, the intrinsic scale parameter of the material, so it cannot simulate the size effect on the micro-nano scale. Some simulations without considering the intrinsic length show that\cite{11,12}, the simulated hardness-depth relationship is deviated from the actual one. In order to better simulate the nanoindentation process, the CPFEM has become a more advanced simulation method.

3. Crystal plasticity finite element method
The microscopic mechanism of plastic deformation of crystal materials is the flow of dislocations along the crystal slip system. The core of the CPFEM is the crystal plasticity constitutive model, that is, the crystal plasticity theory based on deformation mechanisms such as slip and twinning. Crystal plasticity constitutive model can be divided into phenomenological type and mechanism type. The difference between the two is whether the shear strain rate is related to the movable dislocation, but both include mechanisms such as crystal elastic anisotropy and dislocation slip. The dislocation slip mechanism uses plastic shear strain to describe the dislocation movement in the slip system, and then with the help of statistics, the microscopic discontinuous movement is accumulated into a macroscopic continuous plastic deformation process, and finally the micro mechanism of the material is connected with the macro mechanical response.

The field of crystal plasticity was first pioneered by Taylor, Elam, Schmid, Orwan and Polanyi. Taylor and Elam\cite{13} found that the plastic deformation of face-centered cubic crystal aluminum occurs in a discontinuous slip system. Schmid\cite{14} proposed the famous Schmid law, that is, the starting condition of plastic deformation is that the shear stress on a certain slip system reaches a critical value. Orwan\cite{15}, Polanyi\cite{16} and Taylor\cite{17} independently proposed the dislocation movement viewpoint of metal plastic deformation. Taylor proposed single crystal plastic kinematic equations and rate-independent constitutive relations. Hill and Rice\cite{18} concluded that the plastic deformation of a single crystal is a dislocation movement in a specific slip system, and gave a strict mathematical description of the geometry and kinematics of the plastic deformation. In the following decades, Asaro\cite{19,20}, Asaro and Rice\cite{21}, Peirce and Asaro\cite{22}, Needleman and Tvergaard\cite{23} have made great contributions to the development of crystal plasticity theory.

Since the stress and strain of the crystal is established on the shear of the slip system, it provides effective characterization of the stress component distribution, the changes of the plastic zone and the changes of the various hardening mechanisms, and the simulation results are more realistic and accurate than the general elastoplastic model. The CPFEM is a simulation method that has been proven to be able to effectively describe the macro mechanical response of the ISE.

4. Simulation of nanoindentation of ion-irradiated materials
The finite element method of nanoindentation has been widely used to study various materials, and in recent years there have been finite element method simulations for the nanoindentation test of ion-irradiated materials\cite{11,12,24,27}. The damage distribution of ion irradiation in the material is not uniform, which leads to depth dependent hardening. In view of the characterization of non-uniform distribution defects of ion irradiation, there are currently two methods. One method is to artificially layer the damaged area of ion irradiation. For example, a fine division of the irradiation area of 316 stainless steel irradiated by bivalent helium ion according to the depth is carried out\cite{25}, the irradiation damage amount of each layer is assigned, and a smooth gradient damage-depth distribution is formed. Another method is to refer to damage-depth data\cite{26,27}, or use software such as SRIM to calculate radiation damage\cite{28}. For example, in the simulation of single crystal copper ion irradiation nanoindentation\cite{56}, the distribution parameters of the defect density in the SRIM code are determined by the hardness-depth relationship curve after the irradiation. Compared with the phenomenological
display of damage-depth images, the defect density-depth relationship is more conducive to the further analysis of the mechanism of radiation mechanical effects.

The expansion of the plastic zone of the ion-irradiated material is more complicated. Understanding the evolution of the plastic zone during indentation is very important to explain the hardening mechanism. The general theoretical model ignores the interaction between the plastic zone and irradiation. The finite element simulation of crystal plasticity of 316 stainless steel irradiated with bivalent helium ion of different energy [25] found that as the ion energy increases, the plastic zone shrinks. The simulation of tungsten exposed to plasma [12] and the simulation of copper exposed to ion [26] also found this phenomenon. The explanation for this is that irradiation defects hinder sliding dislocations. Therefore, proper consideration of the influence of radiation hardening on the shape and expansion of the plastic zone can be used to better establish the ion-irradiated hardening model.

Finite element simulation of crystal plasticity can effectively help understand the macro-mechanical response of different hardening mechanisms. There are three hardening items for irradiated single crystal material: SSD hardening item, GND hardening item and irradiation defect hardening item. When plastic deformation occurs, the interaction of dislocations and defects leads to annihilation of defects, and SSDs and GNDs will continue to expand with the indentation process [26]. In addition, the GND hardening term is one order of magnitude larger than the radiation defect hardening term, and thus is the dominant factor in the size effect.

5. Conclusions
This article briefly reviews the nanoindentation technology to measure the mechanical properties of ion-irradiated materials and related issues of finite element simulation. This field is a cross-field that combines ion irradiation, nanoindentation, finite element method and other aspects. CPFEM provide a mechanism explanation at the microscopic level such as the generation and expansion of the plastic zone and the influence of the hardening mechanism. Therefore, it is an effective method for the simulation of nanoindentation of ion-irradiated materials. However, the field is still in its infancy at present, and there is little research on the evolution of dislocations. Research in this field can promote the development of the evaluation and screening of the mechanical properties of ion-irradiated materials.

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