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A mechanistic model for depth-dependent hardness of ion irradiated metals

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HIGHLIGHTS

- A model is proposed for the depth-depdendent hardness with ion irradiation effect.
- FEM is performed for the nano-indentation process of ion irradiated stainless steels.
- Theoretical results match well with different sets of experimental data.

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ABSTRACT

A mechanistic model was developed for modeling the depth-dependent hardness in ion irradiated metallic materials. The model is capable of capturing the indentation size effect, ion irradiation induced damage gradient effect, and effect of unirradiated region acting as a soft substrate. A procedure was developed and described in detail to parametrize the model based on experimentally obtained hardness vs. indentation depth curves. Very good agreement was observed between our model predictions and experimental data of several different stainless steels subjected to various ion irradiation conditions. In addition, two hardening mechanisms are revealed in the new model. One is the well-known indentation size effect arising from the creation of geometrically necessary dislocations as the indenter pierces into the materials. The other is the irradiation hardening due to the presence of irradiation-induced defects. As a function of indentation depth h, the hardening due to indentation size effect is described by $\overline{h}^*/h$, while the hardening due to irradiation first follows a power law form Ph^n, then changes to $Z/h - Q/h^3$, where $\overline{h}^*$, P, n, Z and $Q > 0$ are constants. This transition occurs at the indentation depth when the plastic zone reaches the end of the irradiated layer.

1. Introduction

Irradiation-induced damage is one of the major safety threats to the nuclear industry. Full understanding of irradiation-induced material degradation is vital not only to the development of new materials for the next generation nuclear reactors, but also to the extension of the operating lifetimes of the current fleet of nuclear reactors.

Studying the mechanical behavior of metallic materials subjected to neutron irradiation has long been a challenging problem due to the limited availability of neutron sources, high radioactivity of irradiated samples, and long experimental period and high cost. As an alternative, ion irradiated samples have often been used as surrogates to study irradiation damage in metallic materials, because ion irradiation not only induces defects that are similar to those induced by neutron irradiation [1–7], but also has many advantages over neutron irradiation, namely, more availability of ion sources, low radioactivity of irradiated materials, reduced costs and irradiation times, controllable irradiation conditions and the possibility for co-implantation of various kinds of irradiation particles [8–10].

Compared to neutron irradiation, ion irradiation does have some

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limitations. Chief among them is that ion irradiation can only penetrate a very limited depth (a few micrometers) into the sample, and the resulting defect distribution within this irradiated layer is often non-uniform. This makes it almost impossible to fabricate irradiated samples for traditional mechanical tests such as torsional and tensile tests [8–12].

However, the fact that ion irradiation creates a thin surface layer with non-uniformly distributed defects makes ion irradiated samples ideally suited for indentation tests [13]. Through the continuous stiffness measurement (CSM) technique, the depth-dependent hardness can be directly obtained experimentally [14]. Once the hardness H is measured, the material's yield strength σ_{YS} can be approximately related to its hardness through the empirical formula [7] $\sigma_{\mathrm{YS}} = H/k_{\mathrm{H}}$, where k_{H} is a proportionality coefficient. For most metals, $k_{\mathrm{H}} \approx 3$ [15].

In recent years, numbers of indentation tests have been performed to investigate the influence of ion irradiation on the hardness of metallic materials, including single crystals [12,16], pure polycrystals [17,18], and alloys [7,8,19–27]. Among them, stainless steels, a widely used material in nuclear reactors due to their excellent strength, ductility and corrosion resistance, are the most studied materials [5–7,11,28–32].

For example, Chen et al. [11] irradiated samples made of a solution annealed stainless steel with 3 MeV ion at 673K for up to 3 displacements per atom (dpa). They found that the irradiation-induced defects were primarily dislocation loops of similar size to each other, these defects were non-uniformly distributed in the irradiated region. Huang et al. [7] irradiated samples made of 20% cold-worked 316 stainless steel with 7 MeV ions. They also found that dislocation loops were the primary defects. Their average number density was about 3×10^{22} m^{-3}, and the loop size was a few nanometers. Yabuuchi et al. [5] irradiated samples made of SUS316L stainless steel with 1 MeV ions at 573 K with different irradiation doses, and measured the depth-dependent hardness.

These and other studies on various stainless steels subjected to a wide range of ion irradiation conditions seem to indicate that, similar to neutron irradiation [1–4], ion irradiation induces mainly dislocation loops in stainless steels [5–7]. Furthermore, these studies demonstrated that the material behavior under indentation tests shows similar trends: (1) Similar to indenting unirradiated materials, there is an indentation size effect in ion irradiated materials as well, wherein the hardness is observed to increase with decreasing indentation depth, especially in the sub-micrometer depth regime; (2) There is a damage gradient effect in that hardness generally increases with increasing density of irradiation-induced defects, and eventually reaches an upper limit with further increase of the irradiation dose; (3) There is a soft substrate effect, namely, there exists a threshold indentation depth beyond which the hardness vs. depth profile changes significantly, signaling the fact that the plastic zone induced by the indenter has extended deep into the unirradiated material. For stainless steels, this threshold value is about one-tenth to one-fifth of the thickness of the irradiated layer.

Several models have been proposed to explain the experimental data, and to understand the fundamental mechanisms related to the depth-dependent hardness in ion irradiated materials [32–37]. For instance, the Nix-Gao model [33,34] has been used to explain the indentation size effect. The damage gradient effect is accounted for by the non-uniform distribution of irradiation-induced defects in Refs. [36,37], while the soft substrate effect is attributed to the competition between the non-uniform distribution of defect density in the irradiated layer and the un-irradiated material acts as a soft substrate [35–37]. In spite of the extensive effort, these existing models still have serious shortcomings.

First of all, the Nix-Gao model [33] was originally developed for homogeneous materials. The depth-dependent hardness predicted by this model is entirely due to the presence of the geometrically necessary dislocations. In ion irradiated material, the irradiation-induced defect will add additional hardening that cannot be captured by using only the geometrically necessary dislocations. Even though some authors have used the Nix-Gao model to fit the experimentally obtained hardness vs. depth curves in ion irradiated materials [5,24], the physical interpretation of the two fitting parameters H_0 and h^* in the Nix-Gao model become questionable, because neither of them contains information about the irradiation–induced defects. Moreover, the Nix-Gao model can only be approximately employed when the indentation-induced plastic zone is within the irradiated layer [28], beyond which the soft substrate effect becomes increasingly important.

Secondly, most of the existing models for irradiation hardening are based on the well-known Orowan model which, strictly speaking, is applicable only when the defect distribution is uniform. So, to apply the Orowan model to ion irradiated materials, where the defects are non-uniformly distributed, the average defect distribution may have to be used [8]. Note that irradiation hardening is primarily caused by the irradiation-induced defects within the plastic zone. When the plastic zone is fully contained within the irradiated layer, the defect density in the plastic zone is rather non-uniform, therefore, the Orowan model needs to reflect the non-uniform defect distribution in order to be applicable to ion irradiated materials with a non-uniform defect density profile [11].

In this paper, a new model is proposed for the depth-dependent hardness of ion irradiated metallic materials. The model is based on the deformation mechanisms during the indentation of ion irradiated materials. The model is capable of capturing the indentation size effect, the damage gradient effect, and the soft substrate effect. Detailed derivation of the model is presented in Section 2. A procedure to parametrize the model is described in Section 3. The parameterized model is then used in Section 4 to simulate the hardness vs. indentation depth curves obtained experimentally on three different stainless steels subjected to various irradiation conditions. Finally, some conclusion remarks are given in Section 5.

2. Model development

During ion irradiation, defects such as dislocation loops and stacking fault tetrahedrons can be created. These irradiation-induced defects act as barriers for the motion of dislocations. Consequently, the yield strength of irradiated materials increases [8]. In general, such irradiation hardening depends on the density and distribution of irradiation-induced defects as well as the interaction between irradiation-induced defects and existing or newly generated dislocations in the plastically deformed region during the deformation process.

The yield strength of a material is related to the shear stress needed to move dislocations, or the critical resolved shear stress which, in general, can be written as

$$\tau_{\mathrm{CRSS}} \propto \mu b \sqrt{\rho}, \tag{1}$$

where μ is the shear modulus, b the magnitude of Burgers vector, ρ the density of dislocation barriers. To make Eq. (1) an equality, a coefficient is often introduced in front of $\sqrt{\rho}$. This coefficient is commonly called the hardening coefficient. Its value represents the strength of the barrier in preventing the motion of dislocations. Thus, different types of barriers may have different hardening coefficients.

Let the density of dislocations be ρ_{dis} before irradiation, and N_{def} be the number density of the irradiation-induced defects, and their average size be d_{def}. Then Eq. (1) for the irradiated material can be