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Comparison of linear and square superposition hardening models for the surface nanoindentation of ion-irradiated materials

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HIGHLIGHTS

• Linear and square superposition hardening models are compared for ion-irradiated metal.

• Average density of dislocations and defects is considered for the hardening model.

• Results of square superposition hardening model match better with experimental data.

A R T I C L E I N F O

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ABSTRACT

Linear and square superposition hardening models are compared for the surface nanoindentation of ionirradiated materials. Hardening mechanisms of both dislocations and defects within the plasticity affected region (PAR) are considered. Four sets of experimental data for ion-irradiated materials are adopted to compare with theoretical results of the two hardening models. It is indicated that both models describe experimental data equally well when the PAR is within the irradiated layer; whereas, when the PAR is beyond the irradiated region, the square superposition hardening model performs better. Therefore, the square superposition model is recommended to characterize the hardening behavior of ion-irradiated materials.

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In order to study the mechanical behavior of ion-irradiated materials, surface nanoindentation has been widely adopted to characterize the hardening behavior near the irradiated sample surface [1–7]. Considering the limited irradiation depth and non-uniform distribution of defects in the irradiated region, it is not an easy task to theoretically analyze the intrinsic mechanisms resulting in irradiation hardening of ion-irradiated materials [8–11].

When an indenter tip penetrates into the irradiated sample, a plasticity affected region (PAR) would be formed around the indenter tip (as illustrated in Fig. 1). In the PAR, both dislocations and irradiation-induced defects could contribute to the increase of critical resolved shear stress (CRSS), i.e. τ_{CRSS}^{dis} and τ_{CRSS}^{def} . To characterize the hardening behavior induced by different obstacles,

there are generally two superposition models for CRSS, namely, linear superposition model (or say Model I) and square superposition model (or say Model II). Thereinto, the linear superposition model has been widely applied in the framework of crystal plasticity theory considering neutron irradiation effect, which can effectively characterize the increase of yield stress induced by different kinds of obstacles [12]. When the strength of obstacles is at the same level, it has been indicated that the square superposition model is valid to analyze the hardening behavior [13,14]. However, it is also proved that both of these two models can offer a good fit of yield stress considering the hardening contribution of dislocations, dislocations loops and clusters for neutron-irradiated Fe-Cr model alloys [15]. In this work, the rationality for the application of linear and square superposition models to describe the hardening behavior of ion-irradiated materials will be

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Fig. 1. A schematic diagram for the surface nanoindentation of ion-irradiated materials. The depth of irradiation region is L_{d} , and the plasticity affected region is considered as a hemisphere with radius *R*.

systematically analyzed through comparing the numerical results of proposed models with four sets of experimental data [2,16–18].

Considering the contribution of dislocations and irradiationinduced defects, the CRSS for the linear and square superposition models can be respectively expressed as

$$\tau_{\text{CRSS}}^{\text{irr}} = \begin{cases} \tau_{\text{CRSS}}^{\text{dis}} + \tau_{\text{CRSS}}^{\text{def}} & \text{Model I;} \\ \sqrt{\left(\tau_{\text{CRSS}}^{\text{dis}}\right)^2 + \left(\tau_{\text{CRSS}}^{\text{def}}\right)^2} & \text{Model II,} \end{cases}$$
(1)

where $\tau_{CRSS}^{dis} = \mu b \alpha \sqrt{\rho_{dis}}$ and $\tau_{CRSS}^{def} = \mu b \beta \sqrt{N_{def}} d_{def}$. μ and b are the shear modulus and magnitude of Burgers vector, respectively. α and β respectively denote the dislocation and defect hardening coefficient. ρ_{dis} and \overline{N}_{def} are respectively the average density of dislocations and defects in the PAR. d_{def} is the average defect size. Taking into account the von Mises flow and Tabors factor [19,20], the hardness with irradiation effect can, therefore, be given as

$$H_{\rm irr} = 3\sqrt{3}\tau_{\rm CRSS}^{\rm irr}$$

$$= \begin{cases} 3\sqrt{3}\mu b \left(\alpha\sqrt{\rho_{\rm dis}} + \beta\sqrt{\overline{N}_{\rm def}d_{\rm def}}\right) & \text{Model I};\\ 3\sqrt{3}\mu b \sqrt{\alpha^2 \rho_{\rm dis} + \beta^2 \overline{N}_{\rm def}d_{\rm def}} & \text{Model II}. \end{cases}$$
(2)

Following the well-known Nix-Gao model [9], the component of ρ_{dis} can be divided into geometrically necessary dislocations ρ_G and statistically stored dislocations ρ_S , i.e $\rho_{dis} = \rho_G + \rho_S$. Meanwhile, $\rho_G = 3/(2bM^3 \tan\theta h)$ is related to the highly localized deformation

$$H_{\mathrm{irr}} = \begin{cases} H_0 \sqrt{1 + \frac{\overline{h}^*}{h}} + AH_0 \sqrt{\frac{\overline{h}^* h^n}{(n+1)(n+3)(h_c^{\mathrm{sep}})^{n+1}}} & (h \le h_c^{\mathrm{sep}}) \text{ Model I;} \\ H_0 \sqrt{1 + \frac{\overline{h}^*}{h} + \frac{A^2 \overline{h}^* h^n}{(n+1)(n+3)(h_c^{\mathrm{sep}})^{n+1}}} & (h \le h_c^{\mathrm{sep}}) \text{ Model II} \end{cases}$$

around the indenter tip, which depends on the indentation depth *h* [9,11]. Note that the expression of $\rho_{\rm G}$ is different from that of Nix-Gao model [9] as a dimensionless coefficient *M* is considered to approximately express the linear relationship between the radius of the PAR and indentation depth [11]. $\rho_{\rm S} = 3/(2b\tan\theta h^*)$ can characterize the bulk hardness H_0 through $H_0 = 3\sqrt{3}\alpha\mu b\sqrt{\rho_{\rm S}}$ and $h^* = 40.5b\alpha^2\tan^2\theta(\mu/H_0)^2$ [9]. θ is the angle between the surfaces of indented materials and indenter.

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(5)

Concerning the distribution of defect density within the limited irradiated region, it has been noticed that: (1) the defect density as a function of irradiation dose is closely related to the type of irradiated materials and defects [21]. For most irradiated metals, it increases nearly linearly with irradiation dose before it gets saturated [22–24]; and (2) irradiation dose tends to firstly increase with irradiation depth, and then rapidly drops to zero after it reaches a peak value at the maximum irradiation depth for ion-irradiated materials [25,26]. Therefore, the non-uniform distribution of defect density [11] can be approximately expressed as

$$N_{\rm def}(x) = \begin{cases} N_{\rm def}^0 \left(\frac{x}{L_{\rm d}}\right)^n & (x \le L_{\rm d}); \\ 0 & (x > L_{\rm d}), \end{cases}$$
(3)

where L_d is the irradiation depth, and x is the distance from the irradiated sample surface. n and N_{def}^0 are the parameters describing the profile of defect distribution ($n \ge 0$) and peak defect density at L_d , respectively. With Eq. (3), one can not only effectively present the dominant distribution features of defect density for ion-irradiated materials, but also dramatically simplify the expression of the hardening model and parameter calibration process.

By assuming the PAR as a hemisphere with radius *R*, one can respectively calculate \overline{N}_{def} when the PAR is within the irradiated region ($h \le h_c^{sep}$) and beyond the region ($h > h_c^{sep}$) [11], i.e.

$$\overline{N}_{def}(h) = \begin{cases} \frac{3N_{def}^{0}h^{n}}{(n+1)(n+3)(h_{c}^{sep})^{n}} & (h \le h_{c}^{sep});\\ \frac{3N_{def}^{0}}{2} \left[\frac{1}{n+1}\frac{h_{c}^{sep}}{h} - \frac{1}{n+3}\left(\frac{h_{c}^{sep}}{h}\right)^{3}\right] & (h > h_{c}^{sep}), \end{cases}$$
(4)

where $h_c^{sep} = L_d/M$ is a critical indentation depth, at which the PAR reaches the boundary of the irradiated region. By submitting Eq. (4) into Eq. (2), one can finally obtain the expression of hardness with ion irradiation effect at different indentation depths, i.e.

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