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Stress relaxation in icosahedral small particles via generation of circular prismatic dislocation loops

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A theoretical model is developed that describes stress relaxation in icosahedral small particles through generation of circular prismatic dislocation loops. It is shown that loop generation is energetically favorable in the equatorial section of the particle, the radius of which is larger than the critical one. The dislocation loop then extends until it reaches its optimal radius which increases with particle size. Both the critical particle radius and optimal loop radius strongly depend on dislocation core energy.

Keywords: Icosahedral small particles; Residual stresses; Stress relaxation; Dislocation nucleation; Disclinations

Small particles made of materials with a face-centered cubic (fcc) crystalline structure often take the form of a polyhedron or prism having fivefold symmetry axes. Such objects are commonly called 'fivefold twinned' or, simpler, 'pentagonal' particles or rods. These nature artefacts were studied intensively over the last fifty years, but still demonstrate new and unusual properties [1–6]. It was also shown that the fraction of pentagonal particles in observed ensembles of nanoparticles of fcc metals and semiconductors can be large, see, for example, special studies [3] on gold nanoparticles.

It is well known that pentagonal rods and particles are subjected to residual mechanical stresses and store strain energy which is proportional to the particle volume. Nowadays there exists a number of models that explain the formation process and the physical properties of pentagonal small particles [1,7–11]. The models based on the disclination approach [7–9] seem to be the most natural and convenient ones for the quantitative description of the crystal lattice distortions in the pentagonal particles. The residual stresses and the strain energy can relax in the pentagonal particles through different mechanisms involving the generation of various crystal lattice defects such as dislocations, disclinations, low-angle grain boundaries and microtwins, the formation of open gaps, lattice mismatched layers and inclusions, surface whiskers, *etc.* [6,9,12–24]. Some of these mechanisms first predicted theoretically (see, for example, Refs. [12,13,15]), later received experimental confirmations. The reason for the manifestation of the variety of stress relaxation modes in pentagonal small particles still remains unexplained. Perhaps some relaxation processes develop consecutively with increasing the particle size, while others occur simultaneously.

What is evident, the onset of stress relaxation in pentagonal particles occurs through the generation of single defects such as a dislocation segment or an individual circular prismatic dislocation loop (CPDL). The conditions for CPDL generation in a pentagonal rod were studied for the first time in Ref. [25]. For equiaxial pentagonal particles, this problem has not been posed until now due to lack of suitable solutions for strain energy of a CPDL in an elastic sphere. Recently, such a solution has been delivered [26]

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and applied to the models of lattice mismatch relaxation via the generation of misfit CPDLs in bulk [27] and hollow [28] core–shell nanoparticles.

The present work is aimed at the analysis of the critical conditions for the generation of CPDLs in icosahedral small particles (ISPs) and at the finding of the optimal parameters for this process.

Consider an ISP in the initial state before stress relaxation. The geometric model of the ISP made of fcc material can be imaged as composed of 20 tetrahedra with {1 1 1}-type faces [8]. When these tetrahedra are glued together, it is required to have six positive wedge disclinations of strength $\omega \approx 2\pi - 10\sin^{-1}\left(\frac{1}{\sqrt{3}}\right) \approx 7°21' \approx 0.128$ to maintain ISP continuity. Wedge disclinations pass through the opposite vertices of the icosahedron [10]. For the sake of simplicity, one can replace the icosahedron with an elastic sphere containing either six discrete disclinations or a distributed stereo disclination which is also known as Marks–Yoffe disclination [8]. Then, the stress state of the ISP of radius a made of elastically isotropic materials is characterized by the following three non-vanishing stress tensor components [8]:

$$\sigma_{RR} = 2A\chi\ \ln(R/a), \quad \sigma_{\varphi\varphi} = \sigma_{\theta\theta} = \sigma_{RR} + A\chi, \tag{1}$$

where $A = \frac{2G(1+\nu)}{3(1-\nu)}$, $\chi = \frac{3\omega}{2\pi} \approx 0.0613$, G is the shear modulus and ν is the Poisson ratio. The hydrostatic stress component σ and the strain energy E_{ISP} of the ISP are given by:

$$\sigma = \frac{1}{3}(\sigma_{RR} + \sigma_{\phi\phi} + \sigma_{\theta\theta}) = 2A\chi\left[\ln\left(\frac{r}{a}\right) + \frac{1}{3}\right], \tag{2}$$

$$E_{\mathrm{ISP}} = \frac{4\pi}{9}A\chi^2 a^3. \tag{3}$$

From the latter formulas, important conclusions can be made. First, the strain energy grows rapidly with the ISP radius, $E_{\mathrm{ISP}} \sim a^3$, and, therefore relaxation processes become highly expected in growing ISPs. Second, the hydrostatic stress is negative in the central region of the ISP, if $R < a\ \exp(-1/3) \approx 0.72a$, and reaches the highest value in the center. Third, the hydrostatic stress is positive in the peripheral region of the ISP, if $R > 0.72a$, and on the surface ($R = a$) biaxial tension equals $2A\chi/3 \approx G/20$, for $\nu = 0.3$. Such high tensile stresses are expected to stimulate vacancy nucleation at the ISP surface and vacancy migration to ISP central region being under high hydrostatic compression. In real ISPs, the cores of six wedge disclinations can serve as the channels for enhanced vacancy pipe diffusion from the ISP surface to its center. Reaching the ISP center, the vacancies coagulate and form either a pore or a prismatic dislocation loop. It seems reasonable that at the beginning of the relaxation process, the vacancies first form the loop which then increases in size and, after reaching some limit radius, transforms into a pore.

In the present short paper, we consider only the first stage of the stress relaxation in ISPs through the formation of vacancy type CPDLs.

The change in the total energy of the system due to the generation of a CPDL is $\Delta E = E_{\mathrm{fin}} - E_{\mathrm{in}}$, where $E_{\mathrm{in}} = E_{\mathrm{ISP}}$ is the total energy of the ISP in the initial state (Fig. 1a) before relaxation that is the strain energy of the distributed stereo disclination, which is an intrinsic defect in the ISP, and $E_{\mathrm{fin}} = E_{\mathrm{ISP}} + E_{\mathrm{CPDL}} + E_{\mathrm{int}}$ is the total energy of the ISP in its final relaxed state (Fig. 1b). Here E_{CPDL} is the self-energy of the CPDL including both strain and core energy terms, and E_{int} is the energy of interaction between the CPDL and the distributed stereo disclination. Thus, the energy change is given by $\Delta E = E_{\mathrm{CPDL}} + E_{\mathrm{int}}$.

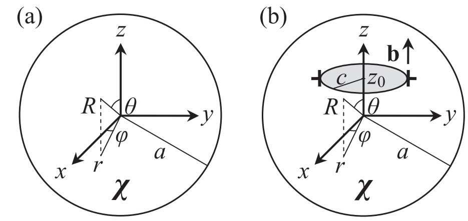

Figure 1. Schematics for the stress relaxation process in an ISP of radius a through generation of a CPDL of radius c with Burgers vector b placed coaxially at the distance z_0 from the ISP center: (a) the initial dislocation free state of the ISP, (b) the relaxed state of the ISP with a CPDL. The Cartesian (x, y, z), cylindrical (r, φ, z) and spherical (R, φ, θ) coordinates are shown.

The self-energy of the CPDL in an elastic sphere with free surface can be written as [26]:

$$E_{\mathrm{CPDL}} = {}^{\infty}E_{\mathrm{CPDL}} - \pi b\int_0^c {}'\sigma_{zz}\Big|_{z=z_0} r dr, \tag{4}$$

where ${}^{\infty}E_{\mathrm{CPDL}}$ is the self-energy of the CPDL in an infinite elastic medium, b is the Burgers vector magnitude of the CPDL, c is the loop radius, ${}'\sigma_{zz}$ is an additional stress of the CPDL, which is caused by a sphere free surface, z and r are coordinates in the cylindrical coordinate system with the origin at the sphere center (see Fig. 1), and z_0 is the distance from the CPDL plane to the sphere center. The first term in Eq. (4) is well known [29,30]:

$$E^{\infty}_{\mathrm{CPDL}} = \frac{Gb^2c}{2(1-\nu)}\left(\ln\frac{8c}{r_c} - 2\right) = \frac{Gb^2c}{2(1-\nu)}\ln\frac{1.08\alpha c}{b}, \tag{5}$$

where r_c is the dislocation core radius, α is a parameter that accounts for the core energy contribution and varies from 0.5 to 5 depending on the material type [31]. The second term in Eq. (4) contains the extra stress ${}'\sigma_{zz}$ [26]:

$${}'\sigma_{zz} = {}'\sigma_{RR}\cos^2\theta + {}'\sigma_{\theta\theta}\sin^2\theta - {}'\sigma_{R\theta}\sin 2\theta, \tag{6}$$

$${}'\sigma_{RR} = -2G\sum_{k=0}^{\infty}\left[A_k(k+1)(k^2-k-2-2\nu)R^k + B_k k(k-1)R^{k-2}\right]P_k(\cos\theta),$$

$${}'\sigma_{\theta\theta} = -2G\sum_{k=0}^{\infty}\left\{-\left[A_k(k+1)(k^2+4k+2+2\nu)R^k + B_k k^2 R^{k-2}\right]\times P_k(\cos\theta) - \left[A'_k(k+5-4\nu)R^k + B'_k R^{k-2}\right]\times\frac{dP_k(\cos\theta)}{d\theta}\cot\theta\right\},$$

$${}'\sigma_{R\theta} = -2G\sum_{k=1}^{\infty}\left[A'_k(k^2+2k-1+2\nu)R^k + B'_k(k-1)R^{k-2}\right]\frac{dP_k(\cos\theta)}{d\theta},$$

where