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The Effect of the Dislocation Elasticity on the Thermal Motion of Attached Particle

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1. Introduction

Results of our recent *in-situ* TEM studies of the thermal motion of liquid Pb nanoparticles attached to fixed dislocations in Al matrix indicate that their motion is affected by a dislocations elasticity [1,2]. Analysis of this effect is presented here. It justifies the method used to determine diffusion coefficients of particles attached to dislocations [1-3].

2. Elastic action of dislocation on the thermal motion of attached particle

In-situ TEM studies show that nanoparticles of liquid Pb trapped by fixed dislocations in Al matrix oscillate in the vicinity of the dislocation lines [1,2], see Fig. 1. It can be explained assuming that the dislocations act on the attached particles as an elastic string, Fig. 2.

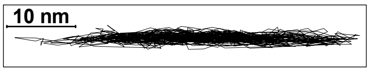

Fig. 1: Trajectory of 15 nm trapped particle recorded at 722 K for 50 seconds. The trajectory is elongated in the direction of dislocation line.

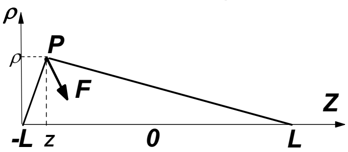

Fig. 2: Action of fixed dislocation segment on attached particle. Point P is its center.

Indeed, transverse displacements ρ of the particle caused by thermal fluctuations produce an elastic restoring force (the arrow $\boldsymbol{F}$ in Fig. 2) due to the linear tension of the dislocation. A projection of this force on the dislocation line (z-axis) causes a repulsion of the particle from closer end of the dislocation. That explains the observed oscillatory motion of the attached liquid Pb particles [1,2]. According to Fig. 2, the displacement of the particle to a point (ρ, z) causes an increase in the dislocation energy $\Delta U = U_o\left(\sqrt{(L+z)^2+\rho^2}+\sqrt{(L-z)^2+\rho^2}-2L\right)$, where $2L$ is the length of the dislocation, U_o is the energy of unit length of the dislocation. $\Delta U = \Delta U(\rho, z)$ defines the elastic energy field determining the elastic restoring force $\boldsymbol{F} = -grad(\Delta U)$. Assuming an axial symmetry, $\boldsymbol{F} = -\frac{\partial \Delta U}{\partial \rho}\frac{\boldsymbol{\rho}}{\rho} - \frac{\partial \Delta U}{\partial z}\frac{\boldsymbol{z}}{z}$, or $\boldsymbol{F} = -f_\rho \boldsymbol{\rho} - f_z \boldsymbol{z}$, where $f_\rho(\rho, z) = \frac{1}{\rho}\frac{\partial \Delta U}{\partial \rho}$ and $f_z(\rho, z) = \frac{1}{z}\frac{\partial \Delta U}{\partial z}$ are the force constants of transverse and longitudinal constituents of the oscillatory motion, respectively. In the assumption $(\rho/L)^2 \ll 1$

$$f_\rho \cong \frac{2U_o}{L(1-\lambda^2)} \quad \text{(1a)} \qquad \text{and} \qquad f_z \cong \frac{2U_o}{L}\frac{\rho^2}{L^2(1-\lambda^2)^2} \quad \text{(1b)}$$

Here $\lambda = z/L$. As $(\rho/L)^2 << 1$, then, $f_\rho >> f_z$, and a frequency of transverse oscillations is much higher than that of longitudinal oscillations. Therefore, the longitudinal motion can be averaged over the transverse oscillations, i.e. ρ^2 in Eq 1b can be replaced by its average value $<\rho^2> = 2kT/f_\rho$ (f_ρ doesn't depend on ρ, see Eq. 1a, then, the transverse oscillations are harmonic, and mean potential energy of the particle is equal to its mean kinetic energy kT). Thus, Eq. 1b transforms to

$$f_z \cong \frac{2kT}{L^2(1-\lambda^2)}. \quad \text{(2)}$$

Equation 1a and Eq. 2 show that f_ρ is determined by the dislocation elastic energy U_oL, and f_z is governed by the energy of thermal motion kT, then, $f_\rho >> f_z$ as the energy of the dislocation elasticity is much larger than the thermal energy.

As attached particles are located mostly in the middle part of dislocations, i.e. $\lambda^2 << 1$ is good enough fulfilled, then, $f_z \approx 2kT/L^2 = \text{const}$, Eq. 2. 1D motion of a Brownian particle in the harmonic potential was considered by Smoluchowski, who had obtained the dependence of mean squared displacement $<\Delta z^2>$ of the particle from its initial position on elapsed time Δt:

$$<\Delta z^2> = 2\sigma_z^2[1-exp(-D_p\Delta t/\sigma_z{}^2)], \quad \text{(3)}$$

where $\sigma_z^2 = kT/f_z$, and D_p is the diffusion coefficient of the particle [4,5]. This equation allows to determine D_p from the 1D trajectory $z(t)$ of the particle. Eq. 3 was used to study the mobility of liquid Pb particles in Al as a function of their size and temperature [1-3].

3. Conclusion

The effect of dislocation elasticity on the thermal motion of a particle, attached to it, is considered analytically. The results of the analysis agree good enough with our experimental observations. It follows from the analysis that the Smoluchowski equation for 1D motion of Brownian particle in the harmonic potential can be used to determine the diffusion coefficients of particles attached to dislocations.

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