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NUCLEATION OF MISFIT DISLOCATIONS BY NANOSCALE IDEAL SHEAR IN SURFACE NANOWIRES AND NANOISLANDS (QUANTUM DOTS)

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Abstract. A new mechanism of misfit dislocation nucleation in surface nanowires and nanoislands (quantum dots) growing on substrates is suggested and theoretically described. The mechanism represents the nucleation of a non-crystallographic partial dislocation whose Burgers vector magnitude continuously grows during the nucleation process. The nucleation occurs by a nanoscale ideal shear that involves collective displacements of atoms of a surface nanowire/nanoisland. It is shown that the new mechanism of dislocation formation in surface nanowires/nanoislands effectively competes with the standard nucleation of a perfect dislocation at a free surface and its further glide towards the nanowire/nanoisland base center.

1. INTRODUCTION

Nanoscale deformation processes and associated transformations of defects in nanostructured and conventional solids represent the subject of intensive research efforts; see, e.g., [1-20]. Of particular interest are such processes in surface nanowires and nanoislands (quantum dots) that grow on substrates and show unique physical (first of all, optoelectronic) properties; see, e.g., reviews [21-23] and book [24]. This interest is motivated by high sensitivity of the outstanding optoelectronic properties of surface nanowires and quantum dots to their structural transformations carried by nanoscale deformation processes. Such deformation processes are commonly driven by misfit stresses generated at interphase boundaries in nanowire/substrate and nanoisland/substrate systems. In particular, misfit stresses in surface nanowires and nanoislands often relax via the formation of misfit dislocations (MDs) causing a dramatic degradation of their functional characteristics; see, e.g., [1-5,18,22-24]. In fact, nucleation of MDs is the most conventional mode of misfit stress relaxation in surface nanowires and nanoislands [1-5,18,22-24], as with flat solid films where MDs serve as typical structural elements crucially influencing the film properties; see, e.g., [25,26]. At the same time, with a rather complex structural geometry of surface nanowires and nanoislands, nucleation of MDs in these nanostructures has specific features [1-5,18,22-24] (differentiating this process from nucleation of MDs in flat films [25,26]). In the context discussed, the knowledge of the conditions and mechanisms for nucleation of MDs in nanoislands (quantum dots) and nanowires is very important from both fundamental and applied viewpoints.

The conventional pathway for MD formation in a surface nanowire or nanoisland involves the nucleation of a dislocation semiloop at the free surface, its subsequent glide towards the equilibrium position at or near nanowire/nanoisland base center; see, e.g., [23] and references therein. This mechanism for MD formation in surface nanowires/nanoisands

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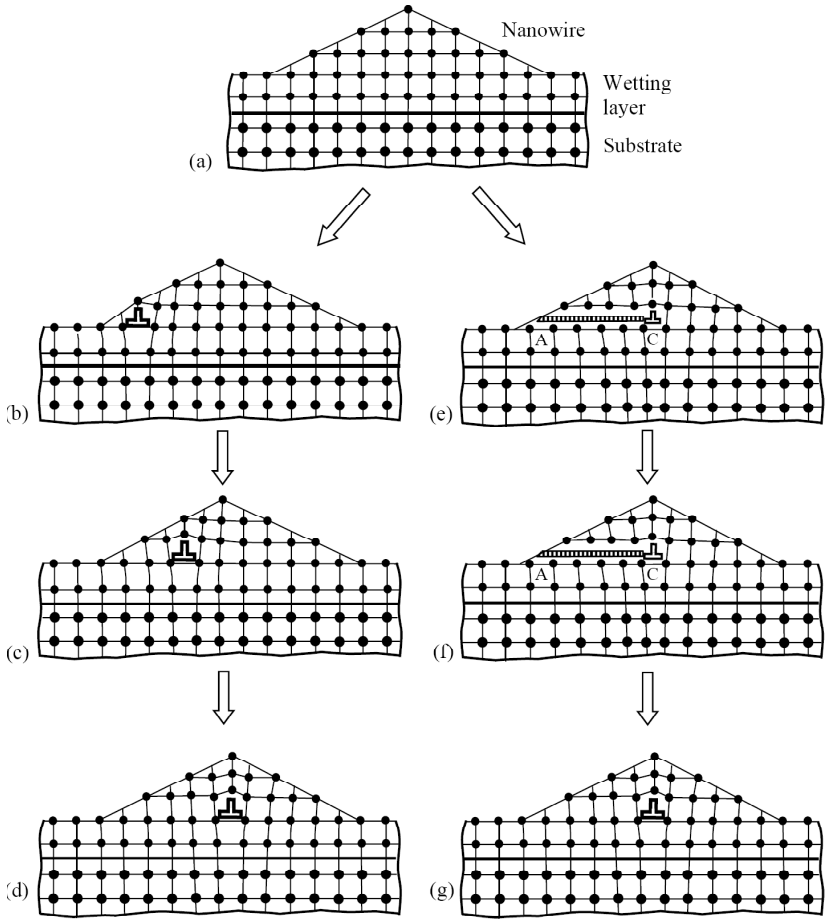

Fig. 1. Micromechanisms for misfit dislocation nucleation in surface nanowires (two-dimensional schematic representation). (a)–(d) Standard mechanism is realized by (a) generation of a misfit dislocation at the nanowire free surface and (b, c) its further glide along the nanowire base to its center where (d) the dislocation stops. (a), (e)–(g) New mechanism involves a nanoscale ideal shear. (a) and (e) A nanoscale ideal shear occurs along plane fragment AC and results in the formation of both a non-crystallographic partial dislocation with an infinitesimal magnitude *s* of the Burgers vector and generalized stacking fault AC. (f) The Burgers vector magnitude *s* continuously increases, and the generalized stacking fault AC evolves. (g) The magnitude *s* reaches the Burgers vector magnitude *b* of a conventional misfit dislocation (perfect lattice dislocation), in which case the generalized stacking fault disappears.

requires that the dislocations overcome a rather high energy barrier, which appears owing to the attraction of dislocations to the free surface. We think that the formation of MDs in surface nanowires and nanoislands can be realized through another, new mechanism with a low energy barrier or even its absence. This mechanism involves the nucleation of a non-crystallographic partial dislocation with a tiny Burgers vector magnitude *s* inside a nanowire/nanoisand (but not at its free surface) and the dislocation evolution through growth of *s* up to the Burgers vector magnitude *b* of a perfect lattice dislocation. The main aim of this paper is to elaborate a theoretical model and give the energy analysis of the new mechanism for dislocation nucleation in surface nanowires and nanoislands (quantum dots) growing on substrates.

2. GEOMETRY OF DISLOCATION NUCLEATION BY NANOSCALE IDEAL SHEAR IN SURFACE NANOWIRES AND QUANTUM DOTS

Let us discuss the specific geometric features of the new relaxation mechanism in nanowires/nanoislands and its difference from the standard relaxation mechanism (Fig. 1). At the beginning of

the standard mechanism action, a MD nucleates at the free surface (Figs. 1a and 1b). Then the dislocation glides towards the nanowire/nanoisland base center along the interphase boundary (Figs. 1b and 1c), where it stops (Fig. 1d). During the standard MD nucleation and glide processes (Figs. 1a–1d), its Burgers vector magnitude *b* is always constant.

The new mechanism for MD nucleation is supposed to pass through two key stages (Figs. 1a, 1e–1g). At the first stage, a momentary ideal (rigid-body) shear occurs along a nanoscale flat fragment AC (Figs. 1a and 1e). The momentary ideal shear is characterized by a small shear magnitude *s* and produces a generalized stacking fault AC of finite nanoscopic length (Fig. 1e). (In the theory of crystals, a generalized stacking fault is defined as a planar defect resulted from a cut of a perfect crystal across a single plane into two parts which are then subjected to a relative displacement through an arbitrary vector ***s*** (lying in the cut plane) and rejoined; see, e.g., [27,28].) The generalized stacking fault ends at a non-crystallographic partial dislocation characterized by a non-quantized (non-crystallographic) Burgers vector ***s*** with quite a small magnitude *s* (Fig. 1e). At the following stage, due to the action of misfit stresses, the magnitude *s* of the dislocation Burgers vector continuously increases and the generalized stacking fault evolves (Fig. 1f). Finally, when *s* reaches the magnitude *b* of the Burgers vector of a perfect dislocation, the generalized stacking fault disappears and the non-crystallographic dislocation transforms into the perfect lattice dislocation (Fig. 1g).

Note that the final state of the nanowire/nanoisland (Fig. 1g) relaxed by the new mechanism is identical to that (Fig. 1d) of the nanowire/nanoisland relaxed by the standard mechanism. Therefore, the difference between the mechanisms may be not identified in conventional ex-situ experiments dealing with relaxed structures. At the same time, the new relaxation mechanism in nanoscale films has its analog – the nanodisturbance deformation mode [29-33] – capable of contributing to plastic flow in various solids. For instance, within the approach [33], a nanoscale generalized stacking fault bounded by a non-crystallographic partial dislocation with a small magnitude *s* of the Burgers vector (Fig. 1e) is called a near-surface nanodisturbance. According to theoretical estimates [33], formation and evolution of near-surface nanodisturbances in free-standing nanowires with face-centered cubic crystal lattices are energetically preferred compared to generation (at a nanowire free surface) and glide of conventional partial dislocations with the Burgers vector b_p. Evolution of a nanodisturbance in a free-standing nanowire under a high mechanical load results in formation of an isolated stable stacking fault within the nanowire section. (When $s = b_p$, a generalized stacking fault in a solid with the face-centered cubic crystal lattice transforms into a conventional or, in other words, stable stacking fault [27,28].) Isolated stable stacking faults (and no dislocations) were experimentally observed in Au nanowires with lateral sizes about 5 nm or smaller [34]. Besides, the near-surface nanodisturbances in surface nanowires/nanoislands on substrates (Figs. 1e and 1f) are similar to "bulk" nanodisturbances experimentally observed [29,35,36] in grain interiors of polycrystals of special titanium alloys called Gum metals. In particular, such "bulk" nanodisturbances were "in situ" observed (by high resolution electron microscopy) during plastic deformation of Gum metals [36]. The discussed experiments indirectly support the suggested representations on nanodisturbances as potential carriers of stress relaxation in surface nanowires/nanoislands on substrates (Figs. 1a, 1e–1g).

3. ENERGY CHARACTERISTICS OF DISLOCATION NUCLEATION BY NANOSCALE IDEAL SHEAR IN SURFACE NANOWIRES AND QUANTUM DOTS

The standard and new (nanodisturbance) relaxation mechanisms (Fig. 1) in surface nanowires/nanoislands on substrates are in competition. To understand how realistic the new mechanism is, we will calculate its energy characteristics and compare them with those of the standard relaxation mechanism in the case of surface nanowires. To do so, let us examine a model nanowire, located on a substrate or a wetting layer, with an infinite length, base width *a* and slope angle α (Fig. 1). The nanowire and substrate are considered to be elastically isotropic solids with identical shear moduli *G* and Poisson ratios ν. The misfit *f* of the parameters a_s and a_{nw} of the substrate and nanowire crystal lattices, respectively, is assumed to be purely dilatational and defined as: $f = (a_s - a_{nw})/a_{nw}$. For clarity, we put $f > 0$.

Note that the 2D model nanowire (Fig. 1) can serve as a first approximation model of a quantum dot. It is a rather conventional approximation in theoretical models of strained quantum dots; for a review, see [23]. In this context, the results of the energy analysis given below can be useful in a de-

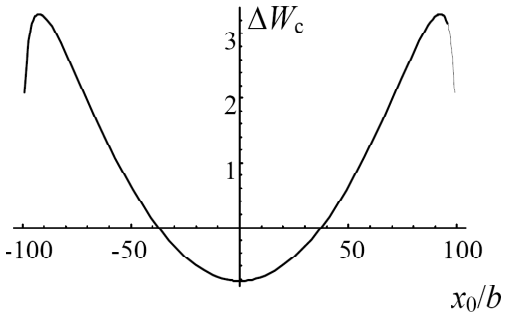

Fig. 2. Dependences of energy change ΔW_c (in units of $Gb^2/[8\pi(1-\nu)]$), associated with the formation of a perfect dislocation in a surface nanowire, on the normalized dislocation coordinate x_0/b.

scription of stress relaxation in both surface nanowires and quantum dots.

Let us examine the critical parameters for the standard formation of a MD through its glide from the nanowire edge along the nanowire base to its center (Figs. 1a–1d). To do so, we calculate the energy change ΔW_c that characterizes standard MD nucleation (Figs. 1a–1d) and is defined as the difference between the energies of the system in its dislocated and initial (dislocation-free) states. The energy change ΔW_c is calculated in paper [37] and depends on the dislocation coordinate x_0. The dislocation coordinate x_0 changes from its initial value $x_0 = -a/2$ at the left nanowire corner to the value $x_0 = 0$ at the nanowire base center. The general formula for ΔW_c is complicated, and so we do not give it here. However, in the partial case $x_0 = 0$ this formula is greatly simplified and can be written as

$$\Delta W_c\left(x_0 = 0\right) = \frac{Db^2}{4}\left(P - \frac{2afQ}{b} + 2\right), \qquad (1)$$

where b denotes the magnitude of the dislocation Burgers vector, $D = G/[2\pi(1-\nu)]$,

$$P = \left(M-1\right)\left[1 - 2\cos^2\alpha\left(M+1\right)\right] - \ln M, \qquad (2)$$

$M = 4b^2/(a^2\sin^2\alpha)$ and

$$Q = \tan\alpha\left(\tan^2\alpha + 2\right)\left(\pi - 2\alpha - \sin 2\alpha\right). \qquad (3)$$

In formula (1), the first term in brackets characterizes the proper strain energy of the dislocation, the second term specifies the energy of its interaction with the misfit stress field, and the third term describes the energy of the dislocation core.

For illustration, the dependence $\Delta W_c(x_0)$ is shown in Fig. 2 in the case of a Ni nanowire on a Cu substrate, for the following typical parameter values: G = 73 GPa, ν = 0.34, b = 0.248 nm, f = 0.026, a = 200 nm, and α = 11°. As it follows from Fig. 2, the formation of a perfect dislocation at the nanowire base center (specified by $x_0 = 0$) is energetically favored ($\Delta W_c(x_0 = 0) < 0$). However, the standard dislocation nucleation at the left nanowire corner and its motion to the nanowire base center require overcoming an energy barrier.

Now we examine the nanodisturbance mechanism for MD nucleation (Figs. 1a, 1e–1g). Let us consider a non-crystallographic partial edge dislocation (with a Burgers vector magnitude s) located at the nanowire base and connected with the nanowire edge by a generalized stacking fault (Fig. 1e). We will use model [37] where the nanowire and substrate are supposed to be cylindrical segments that together compose a cylinder while misfit f is modeled as a continuous distribution of virtual dislocations located at the boundary of the two segments. The energy ΔW_p associated with the formation of the non-crystallographic partial edge dislocation is calculated using the procedure similar to that exploited for the calculation of the energy change characterizing the formation of a partial edge dislocation with a crystallographic Burgers vector [37]. The energy ΔW_p can be written as $\Delta W_p = \Delta W_c|_{b=s} + W_\gamma$, where W_γ is the energy of the stacking fault connecting the partial MD with the left nanowire edge (Fig. 1e). The energy W_γ is given as $W_\gamma = a\gamma(s/b)/2$, where $\gamma(s/b)$ is the specific energy of the stacking fault associated with the partial dislocation having the Burgers vector magnitude s. In order to estimate $\gamma(s/b)$, we take advantage of the following formula that approximates computer simulation results [38] for the specific energy of the generalized stacking fault in Ni:

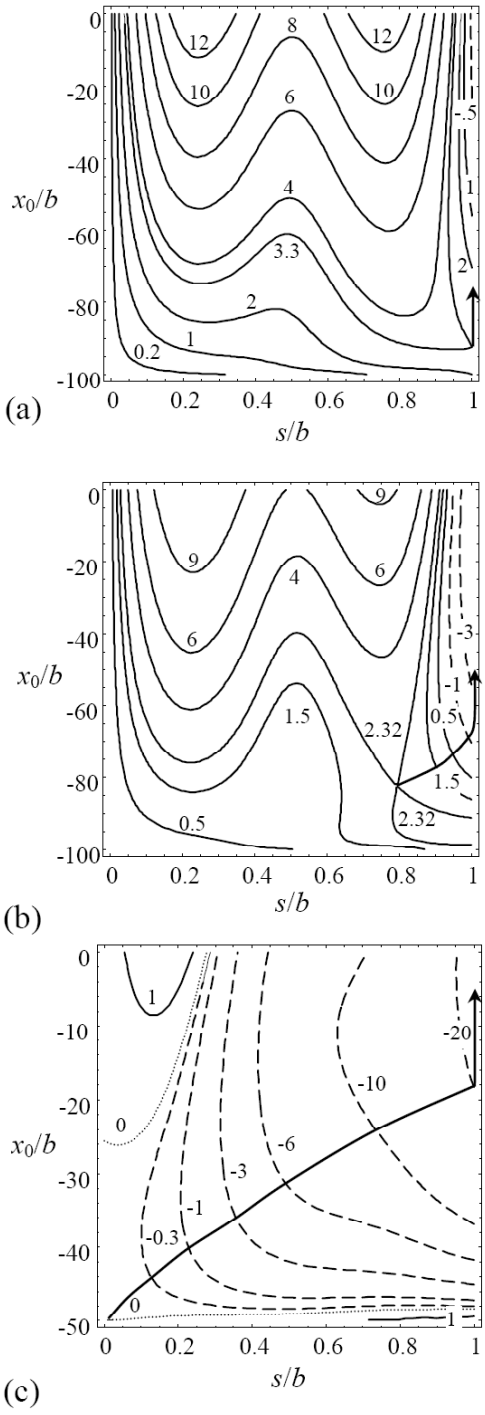

Fig. 3. Contour maps of the energy ΔW_p associated with the formation of a non-crystallographic dislocation and generalized stacking fault in a surface nanowire in the coordinate space (s/b, x_0/b), for (a,b) Ni/Cu system with a/b = 200, α = 11° (a) and 25° (b); and (c) Ni/Ag system with a/b = 100 and α = 11°. The curves with arrows show the preferable trajectories in the coordinate space (s/b, x_0/b), describing evolution of the dislocation. The energy ΔW_p is given in units of $Gb^2/[8\pi(1-\nu)]$.

$$\gamma(s/b)=\begin{cases}\gamma_m \sin\dfrac{2\pi s}{b}, & 0\le\dfrac{s}{b}<\dfrac{1}{4},\\ \dfrac{\gamma_m+\gamma_0}{2}-\dfrac{\gamma_m-\gamma_0}{2}\cos\dfrac{2\pi s}{b}, & \dfrac{1}{4}\le\dfrac{s}{b}<\dfrac{3}{4},\\ -\gamma_m \sin\dfrac{2\pi s}{b}, & \dfrac{3}{4}\le\dfrac{s}{b}\le 1.\end{cases} \quad (4)$$

Here γ_m and γ_0 are the maximum and minimum values of the specific energy $\gamma(s)$ of the generalized stacking fault, that correspond to an unstable and stable stacking fault configuration, respectively; $\gamma_m \approx 0.17$ J/m^2 and $\gamma_0 \approx 0.12$ J/m^2.

To further consider MD formation by the nanodisturbance mechanism, we assume that the magnitude s of the non-crystallographic dislocation Burgers vector and the length $a/2 + x_0$ of the generalized stacking fault can increase separately or simultaneously. In order to theoretically analyze the evolution of a nanodisturbance in the nanowire, we have plotted contour maps of the energy change ΔW_p in the coordinate space (s/b, x_0/b); see Fig. 3. The maps in Fig. 3 are presented for the Ni/Cu and Ni/Ag systems with different values of nanowire base length a, slope angle α and misfit f. As a partial case, these maps give the dependences $\Delta W_c(x_0)$ that characterize the standard nucleation and glide of a perfect dislocation. With these dependences, one can find the energy barrier for the standard nucleation of a perfect dislocation and its glide from the left nanowire corner to the nanowire base center. These dependences can be obtained using the values of ΔW_p at various contours, for s/b = 1.

Fig. 3a shows the contour map of the energy ΔW_p, for the Ni/Cu system with a/b = 200 and α = 11°. In the case of the formation of a nanodisturbance (this case is characterized by increasing both s/b and x_0/b), the evolution of the nanodisturbance can be described by a curve in the parameter space (s/b, x_0/b). As is seen, in Fig. 3a, for both mechanisms of dislocation formation (the glide of a perfect dislocation or the formation of a nanodisturbance), dislocation formation requires surmounting an energy barrier. The contour maps demonstrate that for the case of a nanodisturbance this barrier is minimum if the curve describing the evolution of the nanodisturbance passes through the saddle point (s/b = 1, $x_0/b \approx$ -92). Before reaching this point, the dislocation can move either as a partial non-crystallographic dislocation that simultaneously moves and increases the magnitude of its Burgers vector or as a perfect dislocation, while after reaching this point, the dislocation is energetically preferred to move towards the nanowire base center as a per-

fect dislocation. In any case, in the situation examined, the energy barrier to be surmounted in the case of dislocation formation by the nanodisturbance mechanism is not smaller than that in the case of dislocation formation through the nucleation and glide of a convention perfect dislocation. Therefore, in this situation, the nanodisturbance mechanism of dislocation formation is not more energetically profitable than the standard generation and glide of a perfect dislocation.

Another situation takes place in the case of a model Ni/Cu system with a larger nanowire slope angle α = 25° (Fig. 3b). In this case, dislocation formation also requires surmounting an energy barrier, and this barrier is minimum if the curve describing the evolution of the nanodisturbance passes through the saddle point ($s/b \approx 0.8$, $x_0/b \approx -83$). After passing through this point, the dislocation is favored to move in such a way that it increase both s/b and x_0/b until the magnitude of its Burgers vector reaches that of a perfect dislocation ($s=b$). After that such a perfect dislocation is favored to glide towards the nanowire base center without further changes of its Burgers vector. The evolution of the dislocation after going through the saddle point is shown in Fig. 3b by the curve with an arrow. This curve is drawn for the case where the dislocation evolves in such a way as to provide the maximum magnitude of the energy gradient.

Fig. 3c presents the contour map of the energy ΔW_p for the Ni/Ag system (characterized by the misfit $f \approx 0.16$) with a/b = 100 and α = 11°. As is seen in Fig. 3c, for the considered case, the dislocation can form in the nanowire by the nanodisturbance mechanism in the non-barrier way whereas its formation through the conventional perfect dislocation glide requires surmounting an energy barrier. The evolution of the dislocation for the case of a maximum magnitude of the energy gradient is shown in Fig. 3c as a curve with an arrow. As follows from Fig. 3c, the dislocation is favored to move increasing both s/b and x_0/b until the magnitude of its Burgers vector reaches that of a perfect dislocation ($s = b$). Subsequent dislocation motion is energetically favorable to occur through conventional glide of a perfect dislocation.

To summarize, for small enough values of the misfit f and nanowire slope angles α, the formation of a dislocation in the nanowire through the nanodisturbance mechanism is not preferred compared to its formation as a result of conventional perfect dislocation glide (Fig. 3a). At the same time, for the structures with large enough values of f and/or α (Figs. 3b and 3c), the formation of a dislocation in the nanowire through the nanodisturbance mechanism requires surmounting smaller energy barrier (or even occurs in the absence of such a barrier) than dislocation formation through the conventional glide of a perfect dislocation.

4. CONCLUDING REMARKS

Thus, in this paper a new relaxation mechanism in strained nanowires and quantum dots – the nucleation of non-crystallographic partial MDs with continuously growing Burgers vectors (Figs. 1a, 1e–1g) – has been suggested. According to our energy analysis, this mechanism effectively competes with the standard relaxation mechanism (Figs. 1a–1d) (by MD nucleation at the free surface and its further glide towards the nanowire base center) in a wide range of parameters (size and misfit) of nanowires. In particular, the new relaxation mechanism tends to be preferred over the standard relaxation mechanism in nanowire/substrate and nanoisland/substrate systems with large enough values of f and/or α (Figs. 3b and 3c). In the context discussed, the degradation of the functional properties of nanowires, associated with MD formation, should be experimentally examined and theoretically described in the future, with the features of the new relaxation mechanism taken into account. Of special importance will be the experimental in-situ observations of the MD nucleation events in strained nanowires and quantum dots with various compositions and geometric parameters. Such observations potentially allow one to identify the conditions at which either standard or new mechanism for MD nucleation is dominant. Also, stress relaxation via the formation of non-crystallographic partial MDs in nanowires and quantum dots (Figs. 1a, 1e–1g) is a phenomenon of large fundamental interest, because its analogs can effectively contribute to relaxation processes in various solid structures and thereby influence their physical properties.

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