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Mechanism of formation of the misfit dislocations at the cubic materials interfaces

Yi Wang,^{1,a)} P. Ruterana,^{1,b)} S. Kret,² J. Chen,¹ S. El Kazzi,³ L. Desplanque,³ and X. Wallart³

¹CIMAP, CNRS UMR 6252, 6, Boulevard du Maréchal Juin, 14050 Caen Cedex, France

²Institute of Physics, PAS, AL. Lotnik ów 32/46, 02-668 Warszawa, Poland

³IEMN, UMR-CNRS 8520, BP 60069, 59652 Villeneuve d'Ascq Cedex, France

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High-angle annular dark-field scanning transmission electron microscopy and molecular dynamic simulation are applied to study the misfit dislocations at the GaSb/GaAs interface. In the investigated samples, three types of misfit dislocations have been observed: shuffle and glide set Lomer dislocations and 60° dislocation pairs. The dislocation density tensor analysis is next used to quantify the Burgers vector of misfit dislocations and investigate the misfit dislocation formation mechanism. This work demonstrates that, in these hetero-structures, the dominant mechanism underlying the formation of misfit dislocations is the glide and reaction of 60° dislocations. It is shown that the final structure of each misfit dislocation depends on the Burgers vectors of the initial 60° dislocations. Finally, this analysis points out an approach to determine the local rotation at interface due to mixed type dislocations. © 2012 American Institute of Physics. [<http://dx.doi.org/10.1063/1.4731787>]

Interfacial dislocations have been at the focus of materials research for a long time,^{1–4} and the role of 60° and Lomer (or 90°) misfit dislocations for strain relaxation has already been considered in depth.^{1,5} Recently, it was reported that the epitaxy of highly mismatched III-Sb semiconductors on commercial substrates (Si, GaAs, and GaP) could form Lomer dislocations array which confines the mismatch strain in the interface.^{6–8} Owing to the large lattice mismatch, the critical thickness is expected to be of a few monolayers, subsequently, misfit dislocations are expected to be rapidly generated and relieve the misfit strain. Several types of misfit dislocations including 60° dislocation, Lomer dislocation as well as 60° dislocation closely spaced pair have been reported.^{4,5,9} Up to now, several research groups have reported the reconstruction of the 60° dislocation and Lomer dislocation cores at CdTe/GaAs,² GaAs/Si,^{3,10} Ge/Si,¹¹ and GaSb/Si (Ref. 8) interfaces; however, the proposed structures have been mainly drawn according to transmission electron microscopy (TEM) or scanning transmission electron microscopy (STEM) observations. Moreover, the core structure of the complex 60° dislocation pair, which may be taken as a Lomer dislocation, has been hardly reported. Subsequent to the recent developments in TEM,^{12,13} high-angle annular dark-field (HAADF) imaging or Z-contrast imaging has been applied to determine the precise location and identity of individual atom and clusters,¹⁴ with sub-angstrom resolution.

In this work, we investigate the structure of the misfit dislocations and we determine their formation mechanism at highly lattice mismatched GaSb/GaAs interface using HAADF, along with molecular dynamic (MD) simulation. The formation mechanism is next confirmed by a quantitative Burgers vector analysis using an analytical approach of the dislocation density tensor.

The samples were grown by molecular beam epitaxy (MBE) with a base pressure better than 1×10^{-10} Torr. After the deoxidization of the GaAs substrate at 625 °C under an As flux, a 300 nm GaAs layer was first grown at 580 °C to smooth the surface. Then the Ga and As valves were closed and the temperature was decreased to 485 °C. After an exposure to Sb flux, the (2×4) , (2×8) , or (1×4) surfaces reconstructions of GaAs were generated as monitored by *in situ* reflection high-energy electron diffraction. Then on each of these surfaces, 10 monolayers (MLs) GaSb were deposited. The growth rate was 0.7 ML/s for the GaSb layers with a Sb flux of 2.5 ML/s. Cross-sectional samples were prepared by a standard procedure including grinding, and dimpling and final argon ion beam milling in a stage cooled with liquid nitrogen. The Z contrast HAADF images were acquired using a FEI Titan 80–300 Cubed Microscope equipped with an objective spherical aberration (C_s) corrector operated at 300 kV, along $[110]$ and $[1\bar{1}0]$ zone axis. The C_s in STEM mode is 1.2 mm, thus the probe resolution is 1.36 Å which is below the distance of Ga-Sb dumbbell (1.52 Å) along $[001]$. The relaxation of the GaSb/GaAs hetero-structure was performed by MD simulation using the Stillinger-Weber potential.^{15,16}

Figure 1 shows a high resolution HAADF-STEM image of the GaSb epitaxial layer on GaAs substrate with (2×4) surface reconstruction observed along the $[110]$ zone axis. Since the image intensity in HAADF image is approximately proportional to the square of the atomic number (Z) in 1 s approximation,^{17,18} the bright spots in the epitaxial layer correspond to Sb atomic columns, which is evidently shown by the line intensity profile in Fig. 1(c). As can be seen in Figs. 1(a) and 1(b), the Ga-Sb dumbbell structure is not completely separated; however, the Ga and Sb atoms are clearly identified as shown in Fig. 1(c) by the line intensity profile. Superimposing the atomic model, which is generated by MD simulation, reveals that dislocation 2 is unambiguously a shuffle set Lomer dislocation characterized by a 5/7-atom

^{a)}Email: yi.wang@ensicaen.fr.

^{b)}Email: pierre.ruterana@ensicaen.fr.

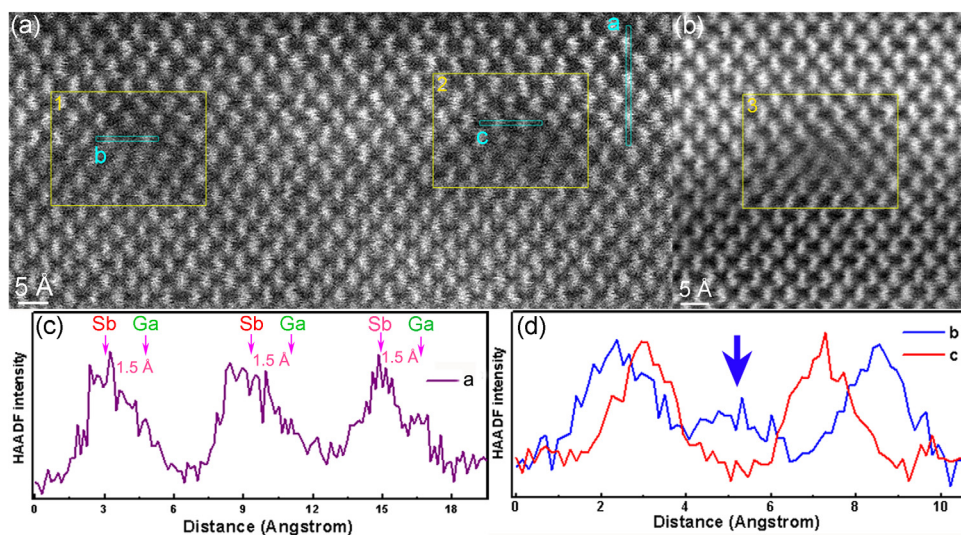


FIG. 1. (a) and (b) High resolution HAADF-STEM images of GaSb epitaxial film on GaAs with (2×4) surface reconstruction; the zone axis is along the $[110]$ GaAs. (c) and (d) The image intensity profiles along the atomic planes indicated by the lines a, b and c, respectively.

ring configuration.^{16,19} Unlike dislocation 2, the higher image intensity in dislocation 1 core center indicates an atomic column inside, as shown in Fig. 1(d). By inspecting the adjacent dumbbells, it can be inferred that the core atomic column is Ga. The presence of a single atom column in dislocation 1 core center yields a glide set Lomer dislocation core with an 8-atom ring configuration.^{16,19} Fig. 1(b) shows an area with a 60° dislocation pair, in contrast to the Lomer dislocation, as can be noticed that the two additional $\{111\}$ planes do not terminate in one atomic ring. In the dislocation core, our HAADF images exhibit comparable information as recent reports on the misfit dislocation by probe corrected STEM which otherwise clearly separated the dumbbells in the epitaxial layer.^{8,20}

Figures 2(a)–2(c) show the simulated HAADF images of the corresponding atomic models obtained by MD simulation with a thickness of 10 nm, using the qSTEM software²¹ for the $C_s = 1.2$ mm of our non probe corrected microscope. The simulated images reproduce the atomic distortion in the dislocation core region and exhibit good agreement with the

experimental HAADF images, which confirms the proposed core configurations. As shown in Fig. 2(d), a line intensity profile (the profile is acquired on the image with larger scanning area, not shown here) along $[001]$ enables us to identify the Sb and Ga atomic columns. Acquiring the line profiles (Fig. 2(e)) across the dislocation 1 and 2 on the simulated images as shown in Figs. 2(a) and 2(b), exhibits similar results as the experimental one (Fig. 1(d)) indicating that the glide and shuffle set dislocations could be identified in our working conditions. Figs. 2(f)–2(h) display the highlighted dislocation core area superimposed with glide and shuffle sets of the Lomer dislocation and 60° dislocation pair atomic model, respectively. On 30 analyzed dislocations, the shuffle set Lomer dislocation with As atomic column core occurs 26 times (86.7%). Then, two Glide set type Lomer dislocations (6.7%) with Ga atomic column core as well as two 60° dislocation pairs (6.7%) have also been observed at this interface.

The relative stability of the Lomer dislocations core has been investigated. Following Hirth and Lothe,²² the energy per unit length of a dislocation is calculated in a cylinder of

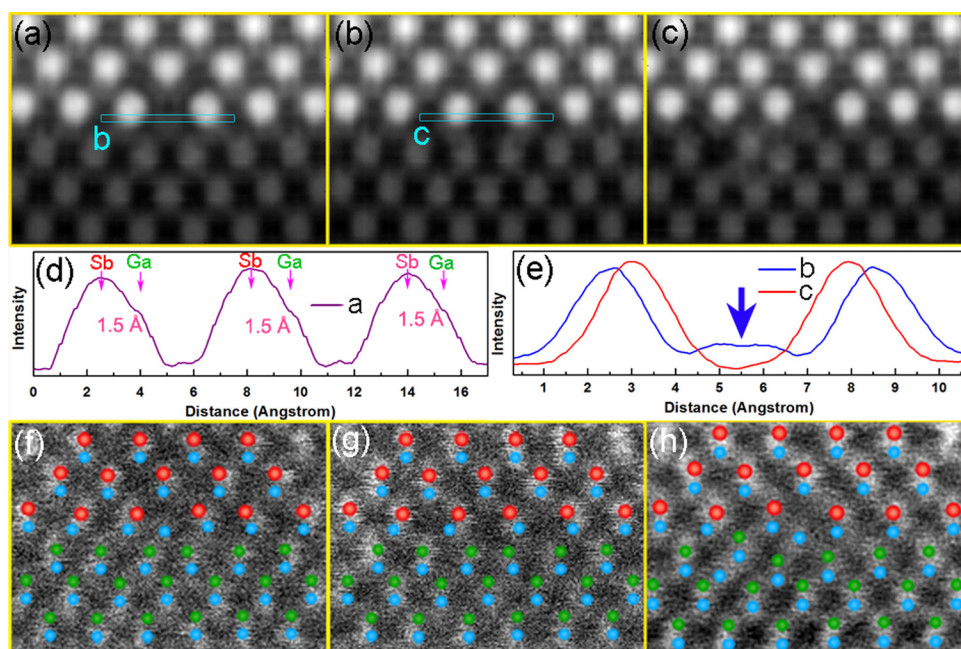


FIG. 2. (a)–(c) The simulated HAADF images. (d) The image intensity profile along $[001]$ atomic columns on a larger area (similar to the line a in Fig. 1(a)). (e) The line intensity profiles across the simulated dislocation cores indicated by lines b and c. (f)–(h) The experimental images superimposed with the atomic models, glide set (1), shuffle set (2) Lomer dislocations, and 60° dislocation pair (3), respectively.

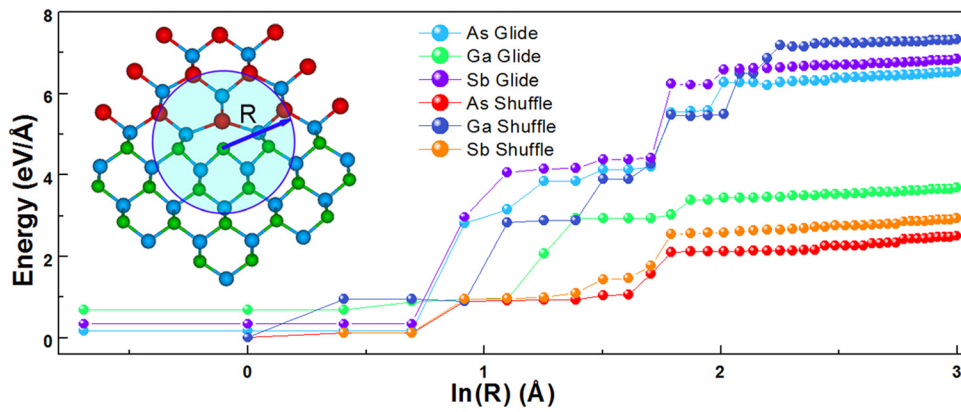


FIG. 3. The energy per unit length (eV/Å), $E_j(R)$ for the different Lomer dislocations plotted as a function of distance from the dislocation core center. The energy is evaluated for a cylinder of radius R around the dislocation core, as schematically shown by the inset.

radius R , as $E(R) = \frac{G|b|^2}{4\pi(1-\nu)} \ln\left(\frac{R}{R_c}\right) + E_c$, ($R \geq R_c$), where G is the shear modulus, ν is the poison's ratio, b is the burgers vector, R_c is the core radius, and E_c the core energy per unit length. Besides the atomic configuration of the interface, the MD calculation also provides the energy of single atom j (E_j). Summing over all the atoms in a cylinder of radius R and length L oriented along the dislocation line (as schematically shown in inset of Fig. 3), one obtains the energy per unit length of a dislocation as $E(R) = \frac{1}{L} \sum_{c(R,L)} E_j$. Figure 3 shows the energy per unit length for the different atomic configurations plotted as a function of distance from the core center. Using a linear fit, the core radius R_c , core energy E_c , and shear modulus G are extracted and summarized in Table I, they correspond to the position when the linear behavior breaks down. Among the calculated atomic configurations, the As core shuffle set Lomer dislocation has the lowest core energy which indicates that it is the most stable configuration. These results are in agreement with the above STEM observations.

In order to determine the misfit dislocation formation mechanism and to quantify the Burgers vector of the dislocations, we performed dislocation density tensor analysis (or Nye tensor analysis²³). The dislocation density tensor characterizes the strength of infinitesimal dislocation at each point in a continuously dislocated crystal and provides a measurement of the Burgers vector.^{24,25} The local Burgers vector is given by the line integral (closed curve around the dislocation) of the lattice distortion tensor²² as well as the surface integral of the dislocation density tensor:²³ $b = \iint_s a \cdot ds = -\oint_l e \cdot dl$, where surface s is bounded by a closed curve l , α and e are the dislocation density tensor and the lattice distortion tensor, respectively. In 2D, the components of the dislocation density tensor α_{xz} and α_{yz} are extracted from the lattice distortion tensor as follows: $\alpha_{xz} = -\frac{\partial e_{xy}}{\partial x} + \frac{\partial e_{xx}}{\partial y}$, $\alpha_{yz} = -\frac{\partial e_{xy}}{\partial x} + \frac{\partial e_{xx}}{\partial y}$; we will simply denote them as α_x and α_y . Experimentally, the lattice distortion

TABLE I. The calculated core energy (E_c), core radii (R_c), and shear modulus (G) of the Lomer dislocations.

	As glide	Ga glide	Sb glide	As shuffle	Ga shuffle	Sb shuffle
R_c (Å)	7.5	6.5	7.5	6	9	6
E_c (eV/Å)	6.2	3.4	6.6	2.0	7.1	2.5
G (GPa)	26.2	22.6	25.1	33.0	26.3	28.5

tensor can be obtained by geometrical phase analysis (GPA) of the micrographs of interest.^{26,27} In fact, the two in-plane components of the tensor field take zero values over the whole region except at the dislocation core position, where they form local peaks, as shown in Fig. 4. Integrating the in-plane component over the dislocation core region we obtain the corresponding Burgers vector component.

Figs. 4(a) and 4(b) show the α_x and α_y components of the dislocation density tensor of a shuffle set Lomer dislocation presented in Fig. 1(a). The bright/dark dots present the deformation maximal area and mark the origin of each extra {111} plane. The corresponding 3D representations of dislocation density tensors at core region are inset into Figs. 4(a) and 4(b), respectively. The distance between the two peaks is less than 1 Å, and the calculated α_x components are very close to the theoretical value for Lomer dislocation ($b = \frac{a}{2}[1\bar{1}0] = 4.0$ Å). Integrating the α_y component in the dislocation core region yields zero; this is consistent with the nature of the Lomer dislocation which is a pure edge

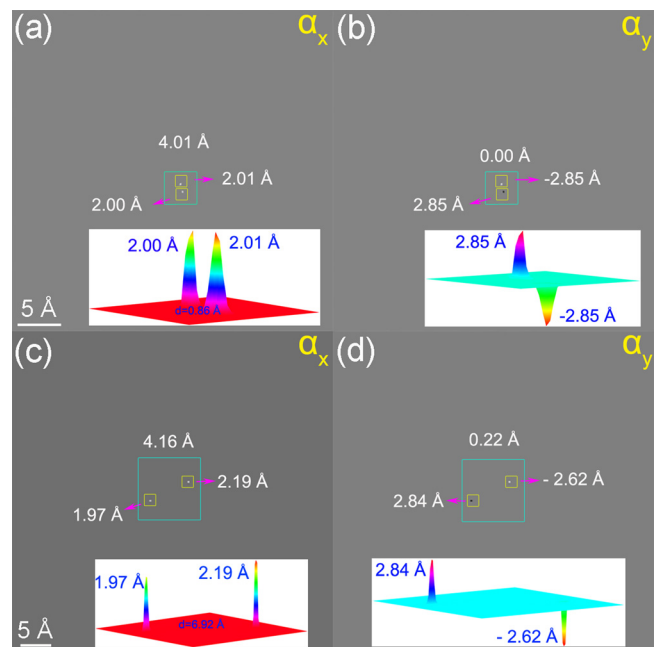


FIG. 4. Dislocation density tensor components α_x (a) and α_y (b) of the shuffle set Lomer dislocation from Fig. 1(a); Dislocation density tensor components α_x (c) and α_y (d) of the 60° dislocation pair from Fig. 1(b); the insets show corresponding 3D representative of the dislocation density tensor α_x and α_y components in the dislocation core region, d is the distance between the two peaks.

dislocation with Burgers vector at 90° to its dislocation line.²⁸ Integrating the two peaks of the Lomer dislocation separately in α_x component we obtain two Burgers vectors corresponding to α_x components of two 60° dislocations (2.0 \AA); in α_y component, the two Burgers vectors have equal amplitude (2.85 \AA) but opposite directions. It can be noticed that for each separate core, the α_y component is 1.4 times larger than the α_x component, as one would expect from the geometrical projection, but in contrast to an earlier work which reported that the α_y should be equal to the α_x .²⁹ As done above for the Lomer dislocation, we have performed the Burgers vectors analysis on a 60° dislocations pair. Figs. 4(c) and 4(d) show the dislocation density tensor images of a 60° dislocation pair from Fig. 1(b) in 2D and 3D views. The two 60° dislocation cores are separated by a distance of 7 \AA . In this case and in contrast to the Lomer dislocation, the α_x and α_y components of 60° dislocations pair are 4.2 and 0.2 \AA , which means that besides the $[1\bar{1}0]$ edge component, we have a small residual edge component along $[001]$ direction. From this HAADF observation, it can be pointed out that one may confuse a 60° dislocations pair with a Lomer dislocation, especially when the two 60° dislocation cores are so close. In both case, one has two intersecting $\{111\}$ planes and drawing the Burgers vector circuit, the 60° dislocations pair will give the same Burgers vector as a Lomer dislocation. However, with the help of the dislocation density tensor analysis, the Burgers vector can be measured precisely and a 60° dislocations pair clearly distinguished from a Lomer dislocation. Similar analyses have been carried out on the samples grown subsequent to (2×8) and (1×4) surface reconstructions. Though they have different ratios for each type of misfit dislocation, they are all characterized by the same feature: each dislocation exhibits two local peaks in the density tensor (as shown in Fig. 4), which is a clear indication that they are generated by the same formation mechanism. In the literature, a number of misfit dislocation mechanisms have been reported: (1) There is a conventional mechanism which is based on the glide of 60° dislocations from the surface and their reaction at the interface;^{1,30} (2) Narayan and Oktyabrsky⁵ reported the formation of Lomer dislocations as well as the 60° dislocations pairs; (3) An alternative rebound mechanism, with a gliding 60° dislocation reaching the interface and next reacting to form a Lomer dislocation and a product dislocation which glides away, has been proposed by Dregia and Hirth;³¹ (4) Chen *et al.*³² implied a model in which a Lomer dislocation may come

from the reaction of a Frank partial dislocation and a 90° Shockley partial dislocation; (5) More recently, Huang *et al.*⁶ and Jallipalli *et al.*³³ assumed that a (2×8) GaAs reconstruction and initial Sb rich growth may lead to direct nucleation of a Lomer dislocations network at the GaSb/GaAs interface (called IMF for interface misfit dislocations⁶). From the above observations, it is clear that a general mechanism should take into account the formation of 60° dislocations pairs at the interface. Therefore, it can be underlined that in this material system where the critical thickness is very small, the relaxation of the misfit strain also proceeds predominantly by the glide of 60° dislocations from the layer surface.³⁴ Subsequently, if the two reacting 60° dislocations have opposite screw components, they will react into a Lomer dislocation (as shown in Fig. 5(b)); otherwise, they are likely to give rise to a 60° dislocation pairs as their parallel screw components prohibit their combination (as shown in Fig. 5(c)). Due to the 7% of 60° dislocation pairs, the mismatch strain in the epitaxial layer is not fully relieved (the measured residual strain by GPA is 5.3%). Moreover, according to other reports,^{5,35} the 60° dislocations pair may not recombine to form a Lomer dislocation even by post annealing: they are likely to split and form stacking faults in the epitaxial layer, as well as probably threading dislocations.

By comparing the measured Burgers vectors with theoretical ones, we are able to determine the local rotation due to the 60° dislocation pair. For instance, in the 60° dislocation pair of Fig. 4, the left side 60° dislocation is perfectly oriented with α_x and α_y components almost equal to the ideal ones, i.e., 1.97 \AA and 2.84 \AA , respectively. However, the right side 60° dislocation, whose α_x and α_y components are 2.19 \AA and 2.62 \AA , yields a screw component of 2.08 \AA . By comparison with an ideal 60° dislocation whose Burgers vector lies along $[10\bar{1}]$ direction, the right side 60° dislocation deviates 4° from the $[10\bar{1}]$ direction, as schematically shown in Fig. 5(c).

In summary, the above observations show that the shuffle set Lomer dislocation with a core made of two As atomic columns is the predominant misfit dislocation at the GaSb/GaAs interface in agreement with MD simulations. From this Burgers vector analysis, it is concluded that the misfit dislocations originate from the glide of the 60° dislocation from the surface and reaction at the interface. Moreover, the dislocation density distribution tensor analysis allows revealing the local rotation of mixed type dislocations.

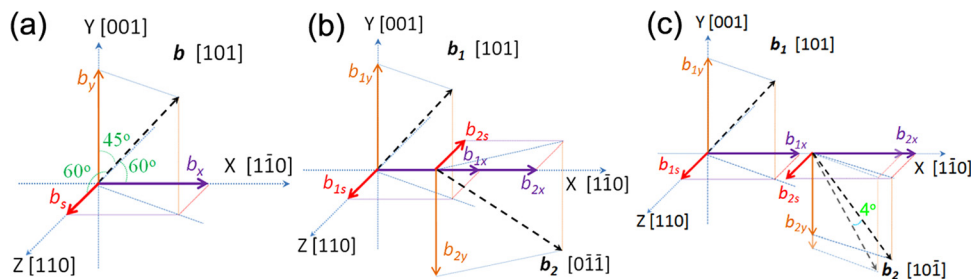


FIG. 5. The schematic geometry diagrams of a 60° dislocation (a) and of the reaction two 60° dislocations in Cartesian coordinate system: the Lomer dislocation (b) and the 60° dislocations pair (c). Here, b indicate the Burgers vector, b_{1s} , b_{1x} , and b_{1y} represent the screw, x , and y directions edge components of dislocation 1, respectively. In (c), the corresponding shade lines indicate the perfect oriented 60° dislocation, 4° is the angle between the rotated 60° dislocation, and a perfect oriented 60° dislocation.

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