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PUBLICATION
Y. Chen and M. Dudley, "Direct Determination of Dislocation Sense of Closed-Core Threading Screw Dislocations using Synchrotron White Beam X-ray Topography in 4*H* Silicon Carbide," *Appl. Phy. Letts.*, **91**, 141918 (2007).

FUNDING
Office of Naval Research
U.S. Department of Energy

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Direct Determination of Dislocation Sense of Closed-Core Threading Screw Dislocations Using Synchrotron White Beam X-ray Topography in 4H Silicon Carbide

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Defects existing in semiconductor single crystal materials adversely affect the device performance fabricated on them. Understanding the defect characters plays a critical role in designing strategies to eliminate or reduce their negative effect. We have used grazing-incidence synchrotron white beam x-ray topography to reveal the dislocation sense (left-handed or right-handed) of the closed-core threading screw dislocations (TSDs) in 4H silicon carbide. Dislocation senses obtained were validated using back-reflection topographs recorded with small Bragg angle. Therefore, the sense of the closed-core TSDs can be unambiguously and non-destructively revealed using either grazing-incidence or "small Bragg angle" back-reflection synchrotron white beam x-ray topography.

Currently no technique can be used to reveal the dislocation sense of closed-core TSDs in commercial 4*H*-SiC wafers in a simple, unambiguous and non-destructive way. We have recently demonstrated two new techniques that can be used to map the dislocation sense of closed-core TSDs in physical vapor transport grown SiC wafers. **Figure 1a** shows a highly enlarged (11-28) grazing-incidence synchrotron white beam x-ray topographic image, containing several closed-core TSDs with Burgers vector 1***c*** (indicated by arrows, the magnitude of ***c*** in 4*H*-SiC is 10.05 Å). It can be observed that an individual TSD appears as a white, roughly elliptical shaped feature, with an asymmetric perimeter of dark contrast that is greatly enhanced on one side or other of the **g**-vector. Clearly, the TSDs visible can be divided into two groups, according to the position of the enhanced perimeter contrast relative to the **g**-vector. One example for each kind is marked by "L" and "R" in **Figure 1a**. The enhanced perimeter contrast is located to the right side of the white contrast for the TSD "L," and to the left side for the TSD "R."

In order to determine the sense of the TSDs, the ray-tracing method has been used to simulate the grazing-incidence topographic images of closed-core TSDs. Simulated grazing-incidence x-ray topographic images of 1***c*** TSDs using the ray-tracing method, taking into account surface relaxation effects, are shown in **Figure 1**. **Figure 1b and 1c** correspond to left-handed and right-handed 1***c*** TSDs, respectively, simulated at a specimen-film distance of 15 cm, where the viewpoint is from behind the x-ray film (see inset on **Figure 1a**). They appear as asymmetric, roughly elliptical white features with perimeters of dark contrast that thicken along one side and at both ends. Such asymmetrical contrast results from surface relaxation effects, which lead to in-plane (***c***-plane) displacements in addition to those along the TSD line direction. For TSDs with line directions slightly inclined to the *c*-axis, both the eccentricity and the inclination angle of the roughly elliptical features change slightly but the enhancement of perimeter contrast along one side persists, acting as an indicator of sign.

Authors (from left) Yi Chen and Michael Dudley

In order to confirm such sense determination of 1*c* TSDs using grazing-incidence topography, "small Bragg angle" back-reflection topography using the basal plane reflection (Bragg angle of 32°, see schematics in **Figure 2a**) was carried out on the same region of the crystal. In the "small Bragg angle" back-reflection geometry, the x-rays penetrate quite deep into the crystal and the TSD again appears as bimodal contrast features. A downward mutual shift of the left-hand column indicates a left-handed TSD while a downward shift of the right-hand indicates right-handed, as schematically illustrated in **Figure 2a**. Vectors $\vec{n}_1$ and $\vec{n}_2$ are the plane normals at either side of the TSD core. Simulated images of left-handed and right-handed TSDs using ray-tracing method, with x-ray absorption being considered, are shown in **Figure 2b**. **Figure 2c** is the "small Bragg angle" back-reflection topographic image of the 1***c*** TSD pair "L" and "R" discussed in **Figure 1**. The downward shift of the left-hand column of the bimodal image of TSD "L" indicated a left-handed sign, while the downward shift of the right-hand column "R" indicates right-handed. This is consistent with our observations from grazing-incidence x-ray topography, based on ray-tracing simulations. Many other 1***c*** TSDs have also been examined and their senses revealed using the position of the enhanced side perimeter contrast on the white contrast features observed on grazing-incidence topographic images. Results are fully consistent with those from the sense of the mutual shift in the bimodal contrast features observed on "small Bragg angle" back-reflection topographic images. Such opposite-sign pair of TSDs may have nucleated at an inclusion. Thus, revealing the sense of TSDs can provide critical information regarding their formation mechanism. This technique can be possibly used in other single crystal materials.

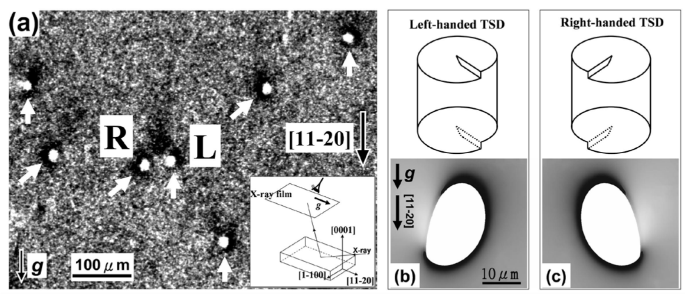

Figure 1. *(a) A highly magnified (11-28) x-ray topograph showing the images of 1c TSDs in 4H-SiC. (b) Ray-tracing simulation of left-handed 1c TSD. (c) Ray-tracing simulation of right-handed 1c TSD.*

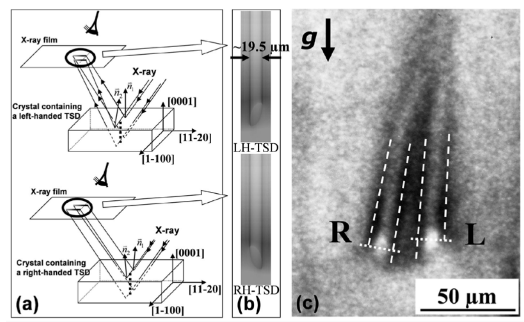

Figure 2. *(a) Schematics showing the mutual shift of the bimodal contrast for a left-handed TSD (upper) and a right-handed TSD (bottom) in "small Bragg angle" back-reflection topography. (b) Simulated images by ray-tracing method. (c) The image of the 1c TSD pair "L" and "R" in Fig. 1(a). LH-TSD: left-handed TSD; RH-TSD: right-handed TSD.*