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Direct Imaging of Dopant Atoms at Dislocation Core in W-doped $NbSi_2$

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Transition metal silicides are attractive candidates for structural applications at temperature higher than ~1000°C, because of their good oxidation resistance and strength at high temperatures. It was shown that, by adding a small amount of W, $NbSi_2$ compound shows significant increase of its high-temperature strength [1], and the strengthening mechanism is believed to be closely related to dislocation-dopant interactions. In the present work, we investigate the dislocation core structure using scanning transmission electron microscopy (STEM), particularly focusing on distribution of W around the dislocations.

In the $NbSi_2$ structure (C40-type), normal dislocations are dissociated into two partial dislocations by accompanying stacking faults. Around dislocation cores, there occurs a significant strain field that causes strong diffraction contrast, which even affect high-angle scattering for HAADF imaging. With this situation, the brightest atomic column cannot be immediately attributed to heavy atom sites; the contrast may not be simply Z-contrast but could be due to residual diffraction contrast (i.e., partially involving Debye-Waller contrast [2]). To overcome this problem, we perform angle-resolved STEM imaging, which provides simultaneous imaging both HAADF/LAADF (Fig. 1). Figures 2 show the HAADF and LAADF images of the dislocation core that extended into two partials with a width of about 2nm. It should be noted in particular that the brightest column appears to be different sites around the partial dislocation cores between the HAADF and LAADF; that is, these sites definitely reveals different angel-dependence of the contrast. On this basis, it is evident that the brightest contrast in HAADF is (mostly) due to chemical Z-contrast representing doped W atoms, and the brightest LAADF contrast at its neighbor sites is mostly caused by Debye-Waller contrast of distorted-columns. From the angle-resolved STEM imaging, we can clearly identify the doped heavy atom positions, even at significantly strained regions.

References

[1] T. Nakano, et al., Acta mater., 48, (2000) 3465-3475.
[2] E. Abe et al., Nature 421 (2003) p. 347, E. Abe et al., Nature Materials 3 (2004) p. 759.
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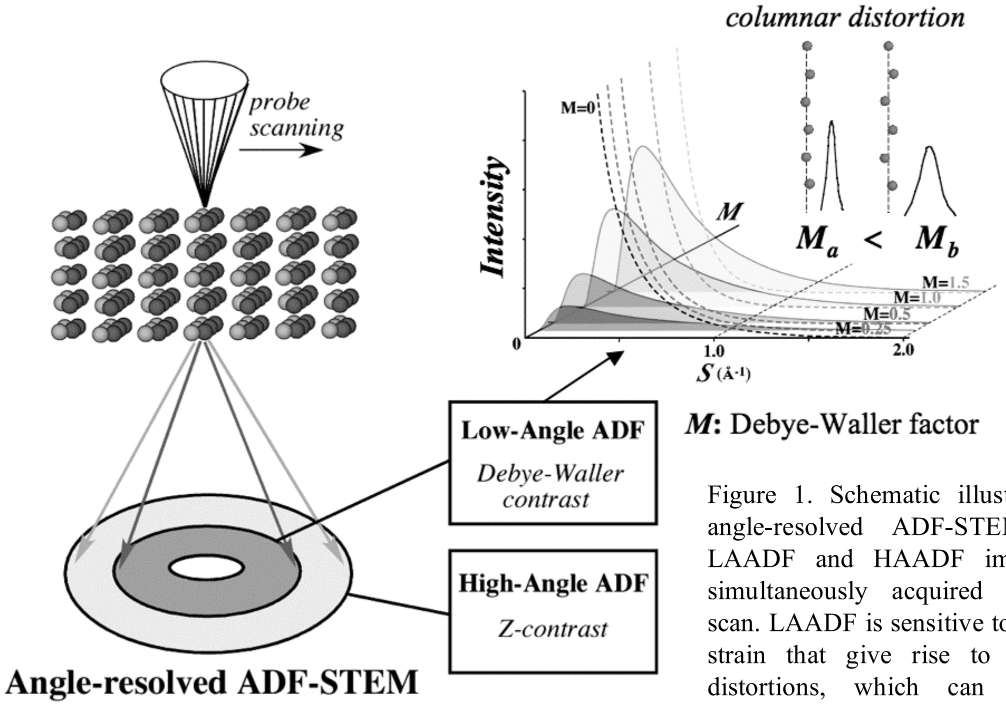

Figure 1. Schematic illustration of angle-resolved ADF-STEM. Both LAADF and HAADF images are simultaneously acquired during a scan. LAADF is sensitive to the local strain that give rise to columnar distortions, which can be well described as *static* Debye-Waller factors.

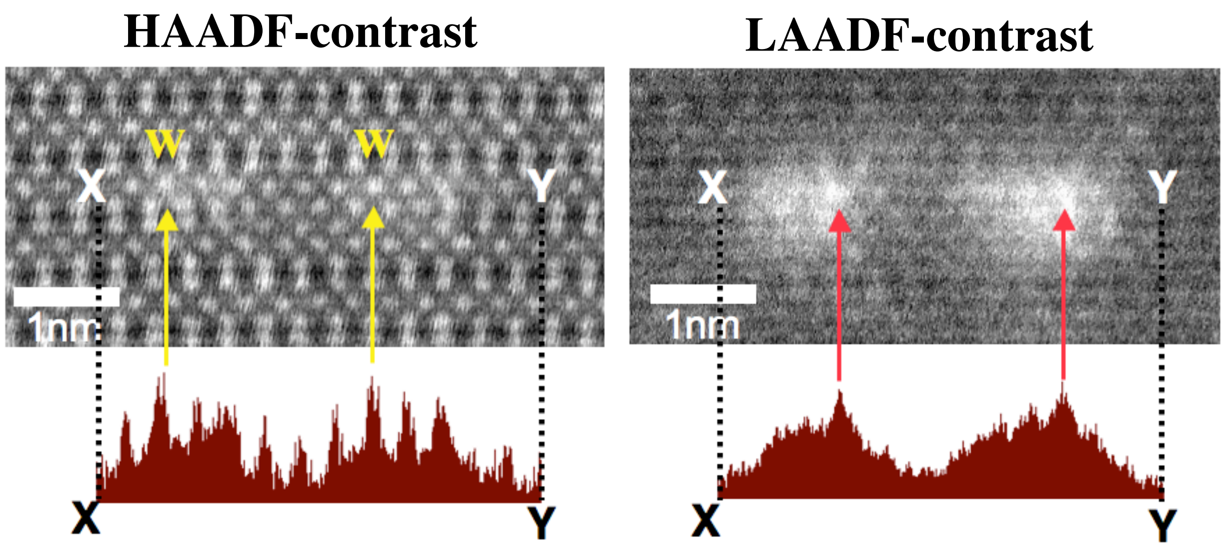

Figure 2. HAADF (left) and LAADF (right) STEM images obtained from the dislocation core of the $NbSi_2$ compound, which are extended into two partial dislocations separated by ~2nm. Note that the brightest columns occur at different sites.