

Dislocation Dissociation and Short-Range Ordering in ZrN

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Transition metal carbides and nitrides generally have a high stacking-fault energy (SFE), due to the bonding in these alloys. This leads to a narrow separation of dissociated dislocations so that direct observation of dislocation dissociation is difficult. Dissociation of $\{111\}\langle\bar{1}\bar{1}0\rangle$ dislocations into Shockley partials in TiC has been reported by Tsurekawa and Yoshinaga [1], and estimates of the SFE range from 130 to 300 mJ/m². The present research was undertaken to determine whether or not dislocation dissociation occurs in ZrN alloy. Sheets of ZrN alloy were annealed at 1200°C and quenched in room-temperature water. Transmission electron microscopy (TEM) was performed on thin foils using a JEOL 2000FXII TEM at 200kV.

As shown in Fig. 1, it was found that perfect $1/2\langle 110\rangle$ dislocations dissociate into two $1/6\langle 112\rangle$ Shockley partial dislocations (arrows) bounding an intrinsic SF in ZrN. This dissociation reaction is the same as that observed in usual FCC alloys and it has not been previously reported for transition metal nitrides with the NaCl prototype structure. All of the dislocations and SF's in ZrN were found to lie on the $\{111\}$ planes, indicating that a possible slip system is $\{111\}\langle\bar{1}\bar{1}0\rangle$. Trace analysis showed that the $1/2\langle 110\rangle$ dislocations contain super-jogs that are not coplanar with the dissociated Shockley partials. The wide separation of the partial dislocations bounding the SF's indicates that the SFE in ZrN alloy is low, with a value of approximately 6 mJ/m². This unusually low SFE can be explained on the basis of a high vacancy concentration in ZrN. Further dissociation of the Shockley partials does not occur, in contrast to the analysis of Kelly and Rowcliffe [2].

The high vacancy concentration in ZrN was confirmed by the appearance of diffuse intensity maxima in electron diffraction patterns, as shown in Fig. 2. Such diffuse intensity comes from the short-range ordering (SRO) of vacancies and nitrogen atoms. When a compound has many point defects, but an insufficient concentration to give long-range ordering, SRO may occur. This ordering causes diffraction effects and a clear example of this phenomenon occurs in metal carbides such as TiC, and VC. In nitrides, evidence for diffuse intensity was found in TiN, but not in VN [3]. Diffuse intensity maxima have not been previously observed in ZrN.

The shapes of the diffuse intensity maxima in ZrN are the same as those found in transition metal carbides. Sauvage and Parthé [4] have analyzed these diffuse intensity maxima theoretically. However, there is a significant increase the diffuse intensity at the $\{1,1/2,0\}$ positions in ZrN (arrows in Fig. 2(a)) as compared to transition metal carbides. Such diffuse intensity maxima at the $\{1,1/2,0\}$ positions have not been previously observed in binary metal carbides and nitrides with the NaCl prototype structure. Similar diffuse intensity maxima were found in Ti₄MoC and these were explained by Ti₄Mo metal-atom ordering, but this is different from ZrN where there is only one metal atom in the phase. Further investigation on the origin of the SRO in ZrN by *in-situ* irradiation in the TEM is currently under investigation [5].

References

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 [5] This research was supported by NSF under grant DMR-9908855.

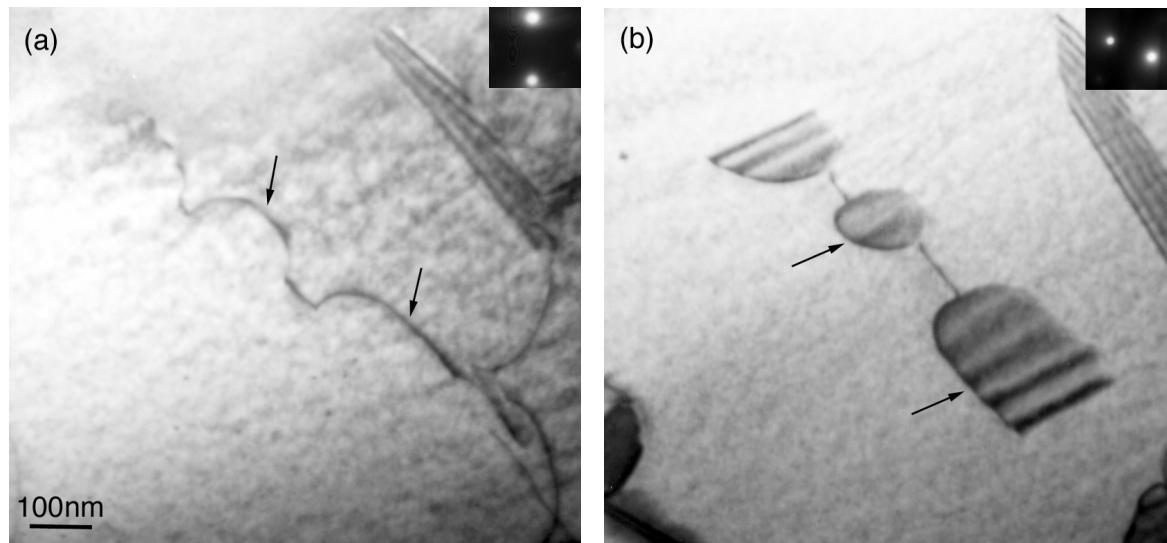


FIG. 1. Bright-field TEM images of dissociated dislocations under different two-beam diffracting conditions: (a) $\mathbf{g}=2\bar{2}0$, $\mathbf{B}=[111]$, $\mathbf{b}=1/6[1\bar{2}1]$ visible (arrows), and (b) $\mathbf{g}=002$, $\mathbf{B}=[100]$, $\mathbf{b}=1/6[\bar{1}\bar{1}2]$ visible (arrows).

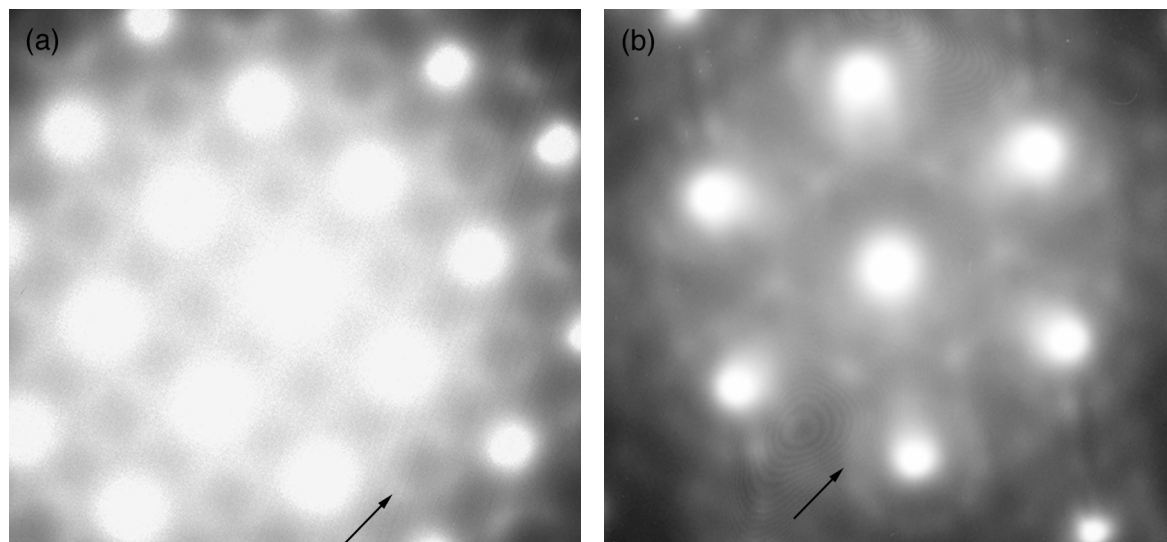


FIG. 2. Diffuse intensity maxima (arrows) in electron diffraction patterns from ZrN observed in two different zone axes due to SRO of vacancies: (a) $\mathbf{B}=[100]$, and (b) $\mathbf{B}=[111]$.