

Coincidence of Reciprocal Lattice Point Model For General Orientation Relationships in Hetero systems

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Crystallographic orientation relationships (OR) have been extensively researched in advanced materials because of their direct influence on interface properties. Most of the prediction methods for the ORs have been applied for dissimilar crystals with only a small lattice mismatch. On the other hand, coincidence of reciprocal lattice point (CRLP) model can be applied to basically all types of crystalline-crystalline hetero systems even with large mismatch [1]. CRLP model can predict not only the most stable OR but also other possible *secondary* ORs between two crystals in three-dimensional space. In this study, CRLP calculations are applied to different metal/ceramic systems to predict the stable ORs based on geometrical coherency.

Two of the most common ORs in cubic/hexagonal structures are determined as OR **A**: (111)[0 $\bar{1}1$]cubic//((0001)[0 $\bar{1}10$]hcp and as OR **B**: (111)[$\bar{1}10$]cubic//((0001)[2 $\bar{1}\bar{1}0$]hcp). OR **B** can be obtained by a 30° rotation of the metal around the [111] direction with respect to OR **A**. CRLP model successfully predicted the experimentally observed ORs in Al/ α -Al₂O₃, Si/ α -Al₂O₃, Al/AlN and Si/AlN. The most stable OR in Al/ α -Al₂O₃ is shown with the maximum geometrical coherency (highest overlapping volume) in Fig. 1a [2]. OR **A** in CRLP matches the epitaxial relationship in Al/ α -Al₂O₃ as observed in high resolution transmission electron microscope (HRTEM) in Fig. 1b. Other preferentially stable *secondary* ORs, **B** and **C**, are also calculated in CRLP in the [111] rotational axis for Al/ α -Al₂O₃ hetero system. At $\Omega = 11^\circ$ OR **C** is identified as: (111)[5 $\bar{1}\bar{4}$]Al//((0001)[$\bar{1}\bar{1}00$] α -Al₂O₃). These *secondary* ORs appear as variants in previous experiments of Al film deposition on α -Al₂O₃(0001). The same most stable OR **A** is also predicted in CRLP for Si/ α -Al₂O₃ hetero system, which is consistent with the most stable OR between Si precipitate and α -Al₂O₃ as shown in the HRTEM image in Fig. 1c [3]. In Al/AlN hetero system, a 3.7° tilt of Al (111) in the [$\bar{1}10$] rotational axis shows a more geometrically coherent OR **B*** than OR **B** in the 2-D CRLP plot (Fig. 2a). This Al(111) tilt on AlN(0001) at the azimuth [$\bar{1}\bar{1}0$]//[$\bar{1}1\bar{2}0$] is shown experimentally in the HRTEM image for liquid phase bonded Al(Si)/AlN hetero interface (Fig. 2b). A unique OR **B*** is identified in CRLP model as: (001)[$\bar{1}\bar{1}0$]Al//((2 $\bar{2}03$)[$\bar{1}1\bar{2}0$]AlN). This suggests a stronger interaction between Al(001) and AlN(2 $\bar{2}03$). CRLP model detects OR **B** as one of the preferential *secondary* ORs in Si/AlN hetero system. The CRLP predicted OR **B** matches the local epitaxial relationship in Si thin film on AlN by pulsed laser deposition. Other metal/ α -Al₂O₃ hetero systems also show good agreement between CRLP calculations and previous experimental findings [2].

CRLP calculations successfully estimate the preferential ORs and their relative stabilities in cubic/hcp structures. CRLP is thus considered to be a powerful tool to predict not only the most stable OR but also other preferentially stable *secondary* ORs for common metal/ceramic systems as experimentally observed in HRTEM studies.

[1] Y. Ikuhara and P. Pirouz, *Microsc. Res. Tech.* 40 (1998) 206.

[2] C. M. Montesa et al., *Mater. Sci. Eng. B* (2010), doi:10.1016/j.mseb.2009.12.023.

[3] C. M. Montesa et al., *Mater. Transac.* 50 (2009) 1037.

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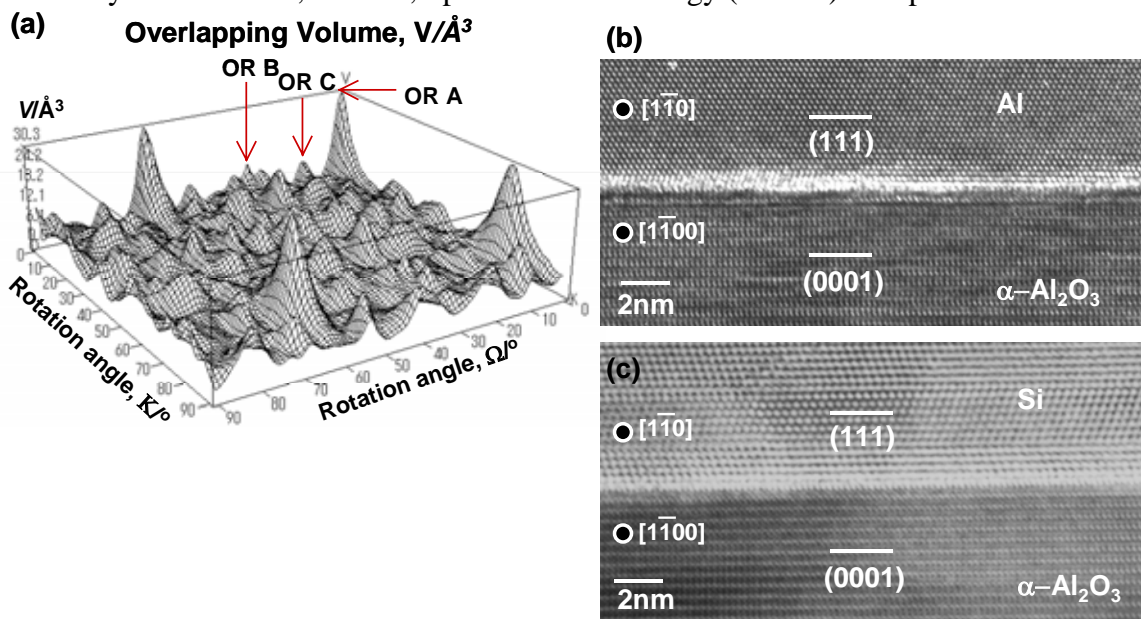


FIG. 1. (a) CRLP 3D profile of Al/ $\alpha\text{-Al}_2\text{O}_3$, which shows the most stable OR A and other preferential *secondary* ORs. (b) HRTEM image of epitaxial Al/ $\alpha\text{-Al}_2\text{O}_3$ by pulsed laser deposition, which shows OR A. (c) An equivalent OR A is shown in the HRTEM image of Si precipitate on $\alpha\text{-Al}_2\text{O}_3$ substrate in liquid phase bonded Al-Si/ $\alpha\text{-Al}_2\text{O}_3$ hetero interface.

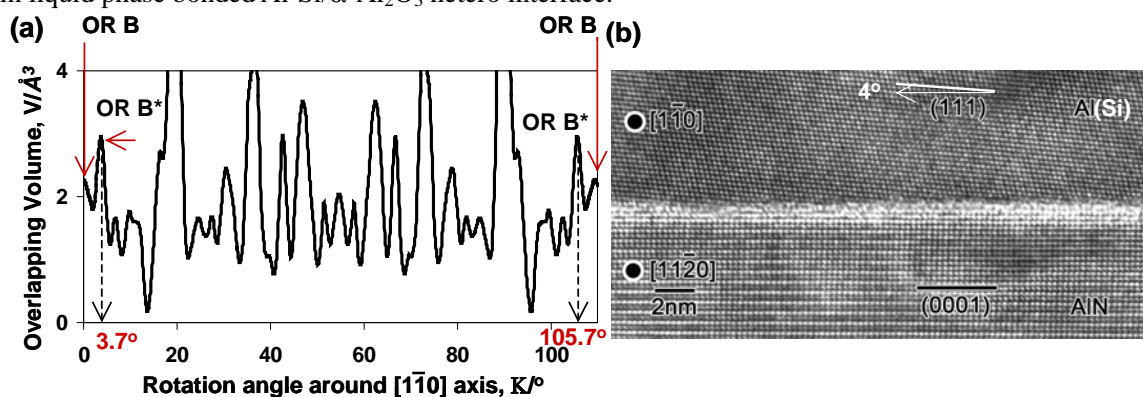


FIG. 2. (a) CRLP 2D plot of Al/AlN hetero system with the more stable OR B*, at the tilt of 3.7° for Al(111), than OR B at zero tilt. Equivalent peaks are seen for OR B* and OR B at $K=105.7^\circ$ and 109.5° respectively. (b) HRTEM image of localized epitaxial area of Al (with trace amount of dissolved silicon), which shows the orientation relationship: $[1\bar{1}0]\text{Al}/[1\bar{1}20]\text{AlN}$, $\sim 4^\circ$ tilt $(111)\text{Al}$ on $(0001)\text{AlN}$.