THE DIRECTIONALITY OF INTERFACIAL CRACKING IN BIMATERIALS

JIAN-SHENG WANG AND GLENN E. BELTZ Division of Applied Sciences, Harvard University, Cambridge, MA 02138

ABSTRACT

Directionality of interfacial cracking resistance in bicrystals has been predicted by a modified Rice-Thomson model and supported by experimental results on $\Sigma 9 \ [110]/(2\overline{2}1)$ Cu bicrystals in Wang and Anderson's recent work. With the intention of extending this work to the behavior of interfacial cracks in dissimilar materials, Rice, Suo and Wang predicted that this directionality also occurs in bimaterials. Reported here are experimental results on Cu/sapphire specimens, which again support the prediction of the theory. A crack along the interface in a Cu/sapphire bimaterial is brittle and decohesion of the interface occurs when the crack propagates in the $[114]_{\text{Cu}}$ direction, whereas it is ductile and dislocation blunting operates if the crack is intended to propagate in the $[114]_{\text{Cu}}$ direction. This finding is significant theoretically and is of helpful in understanding interfacial cracking in composites and film spalling in packaging materials.

INTRODUCTION

It has been well known that the cracking behavior of an interface between crystals depends strongly on its structure. It has been shown only recently, however, that for the same interface the cracking behavior depends also on the direction of the crack propagation. An interfacial crack that propagates in a ductile manner in one direction may undergo cleavage leading to a brittle decohesion in the opposite direction. Thus, the response of a stressed interfacial crack is not only interface structure dependent, but also growth direction dependent.

Intuitively, the cracking directionality is easy to understand. Any process which involves dislocation slip of Schmid type is dependent on the orientation of the active slip planes. For most interfaces, the configuration of the active slip systems at a crack tip is different when the direction of the crack propagation is reversed, leading to a directional dependence of the cracking

The directionality of cracking in bicrystals has been predicted by the Rice-Thomson model [1] and supported by experimental results on $\Sigma 9$ [110]/(221) Cu bicrystals in Wang and Anderson's recent work [2]. With the intention of extending this work to the behavior of interfacial cracks in dissimilar materials, Rice, Suo and Wang predicted that cracking directionality occurs also in bimaterials [3].

In the spirit of testing the idea that the competition between dislocation emission and cleavage decohesion controls the ductile versus brittle behavior of a metal/ceramic interface and that the cracking response is direction dependent, fracture behaviors of interfaces in bimaterials were investigated. Reported here are experimental results on Cu/sapphire specimens.

EXPERIMENTAL PROCEDURE AND RESULTS

Single crystals of copper used in the experiments were grown by a vertical Bridgman technique in an atmosphere of flowing argon gas. Rectangular pieces of 47.6x4.8x2.5 mm were cut via spark-cutting. After mechanically and chemically polishing and cleaning the $(2\overline{21})$ surface of the Cu single crystal was bonded to the basal plane of a commercially-obtained sapphire slide (1 mm thick) by diffusion bonding. The diffusion bonding was carried out in an atmosphere of flowing forming gas (a gas mixture of 20% hydrogen + 80% argon) at 1313 K for 72 hours under a rigid graphite support clamp to maintain a compressive force during bonding. After

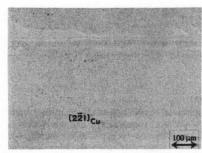


Fig. 1. The diffusionally bonded interface of a Cu/sapphire specimen viewed through the sapphire layer. Pores are seen, indicating small unbonded spots.

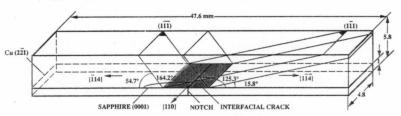


Fig.2. The geometry of the specimen and a schematic presentation of the slip plane configurations at the crack tips of the opposite directions.

bonding the specimen was cyclically annealed to reduce the interfacial stress and remove small grains which sometimes appeared near the interface during bonding. Observations through the optically transparent sapphire layer showed that the quality of the bonding was adequate; the interface was free of any potential reaction products and only a few pores were observed, indicating small unbonded spots (Fig. 1).

A pre-notch was created at the midpoint of the sapphire layer and then the specimen was subjected to a bend load so that an initial crack was produced and run to the Cu/sapphire interface, along which it branched a small amount in both directions, i. e. the $[\bar{1}14]_{\text{Cu}}$ and $[1\bar{1}4]_{\text{Cu}}$ directions. The geometry of the specimen and the slip plane configurations at the crack fronts of the opposite directions are shown schematically in Fig. 2. The pre-cracked specimen was loaded under four-point bending with a screw-driven Instron mechanical testing machine until a nonlinear load versus deflection relation was noted, and then it was unloaded and reloaded several times to enable stable crack propagation. Debonding of the interface at the crack tip, whenever it occurred in either direction, was observed by an optical microscope through the sapphire layer. The energy release rate for debonding, G, was obtained from the load-deflection curve [3]. Slip traces, which indicate dislocation slip on active slip systems in the Cu single crystal, were observed on the polished (110) side surface of the crystal with SEM or optical microscopy.

Five identical specimens were tested in the same procedure. The average value of G was measured to be 5.5 ± 0.5 J/m². Observations showed that in all specimens tested the interfacial crack propagated stably in the $[\overline{1}14]_{Cu}$ direction causing significant interfacial debonding; whereas in the $[1\overline{14}]_{Cu}$ direction plastic deformation occurred, causing crack tip blunting. An example which demonstrates this kind of asymmetrical cracking behavior is shown in Fig. 3. In one particular case the directional effect was profound: in the $[\overline{1}14]_{Cu}$ direction the crack propagated unstably all the way to the end of the specimen causing half of the sapphire layer to detach entirely from the specimen; whereas in the $[\overline{1}\overline{14}]_{Cu}$ direction the crack propagated only a

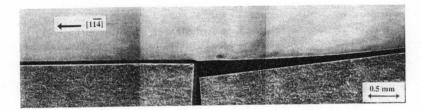


Fig. 3. The side view of a Cu/sapphire specimen after mechanical testing which shows that the crack propagated only in the $[\overline{1}14]_{Cu}$ direction and crack tip blunting occurred in the $[1\overline{14}]_{Cu}$ direction.

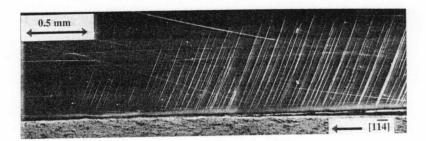


Fig. 4. The dark field optical photograph shows the dense slip lines in the vicinity of the crack which propagated in the $[1\overline{14}]_{Cu}$ direction.

small amount. Dense slip lines on the polished $(110)_{Cu}$ side surface at the vicinity of the crack appeared (Fig. 4), indicating a large amount of plastic deformation. It was identified from the angle of the slip lines that in this case only the (111) slip planes, which make an angle of 125.3° with the crack plane, were active. In the opposite direction the slip lines were much less dense, and again, only the (111) system was active which, in this direction, makes an angle of 54.7° with the crack plane.

As we will see in the next section of the paper, calculations by the modified Rice-Thomson model show that in the $[1\overline{14}]_{Cu}$ direction, dislocations are easier to nucleate on $(1\overline{11})$ planes; in contrast, in the $[114]_{Cu}$ direction only $(1\overline{11})$ planes with the inclination angle of 164.2° may be activated and dislocation nucleation on $(1\overline{11})$ planes is very difficult. The slip lines observed in this direction is thus not produced by the crack tip emitted dislocations. Rather, they are induced by internal dislocations. The controlling process for the crack propagation in the $[114]_{Cu}$ direction is indeed interfacial debonding, while in the $[11\overline{4}]_{Cu}$ direction the controlling process is dislocation slip: a strong directionality of interfacial cracking in the Copper/sapphire interface as that predicted by the modified Rice-Thomson model. Now, let us turn to the model.

DISCUSSION

The directionality of interfacial cracking might be partly understood in terms of the competition between dislocation emission from the crack tip and cleavage, a concept quantified initially by Rice and Thomson [4] to deal with ductile versus brittle response in crystals. An extended Rice-Thomson model was proposed by Rice, Suo and Wang [3] to treat the situation

involving a straight edge dislocation emanating from the tip of a crack lying on a metal/ceramic interface. In the model the energy release rate for dislocation emission from the crack tip, G_{disl} , and the energy release rate for debonding of the interface, G_{cleav} , were compared. If $G_{disl} < G_{cleav}$, dislocation emission was assumed to occur before interfacial decohesion, blunting the tip of the crack; the interface was predicted to be ductile. On the other hand, if $G_{disl} > G_{cleav}$, then decohesion was assumed to occur before dislocation emission and the interface was said to be intrinsically brittle. While G_{cleav} is relatively insensitive to the structure of the interface [2], G_{disl} , being mainly determined by the resolved shear stress on the slip plane, may change dramatically with the change of the inclination angle of the slip plane with respect to the crack plane. This occurs when changing the direction of crack growth in asymmetrical orientation like in Fig. 2, causing the directionality of interfacial cracking.

There are two levels of approaches in deriving the energy release rate for dislocation emission from a crack tip: an older approach following [1], which treats the dislocation as an elastic line singularity in a continuum solid; and a new approach [5], where the dislocation is treated in the Peierls-Nabarro sense. At present, both approaches can only treat the situation where the crack front lies in a slip plane. One advantage of the Peierls-type approach is that it avoids the use of a core cutoff parameter, a necessity in the singular dislocation line approach and

the vaguest parameter in elastic dislocation theory.

In the extension of the theory to the metal/ceramic interface, both approaches regard the ceramic side of the interface as an elastic solid, in which no dislocation activity takes place; only in the metal side is dislocation activity assumed to be possible. With this assumption, a treatment similar to that for dislocation emission from a crack tip in single crystals may be adopted and the only modification needed is to introduce a new parameter: the atomic scale local phase angle, ψ' , a measure of the ratio of local mode II to mode I conditions on a distance of atomic length scale from the crack tip, and is defined by

$$\psi' = \psi - \varepsilon \ln(h/b). \tag{1}$$

Here ψ is the loading phase angle, depending on the loading conditions and also on the elastic combination of the bimaterial, ε is the oscillatory index characterizing the oscillatory stress field near the tip of an interfacial crack, h represents a characteristic length scale of the specimen and b, as usual, is the magnitude of the Burgers vector. Limited by the length of the paper, we are not going to the details of the model; only the major conclusions are given below. Readers who are interested in are referred to Rice, Suo and Wang [2] for the singular dislocation line approach and Rice [5] and Beltz and Rice [6] for the Peierls approach.

Considering joined isotropic solids under in-plane loadings, so that K_{III} =0 and the near tip field is fully characterized by a complex stress intensity factor K, Rice, Suo and Wang [2] derived the energy release rate needed for a straight edge dislocation emanating from the crack tip

in a metal/ceramic interface as

$$G_{disl} = \frac{\mu_1 b^2}{(1 - \nu_1)(1 - \alpha)r_c} \left\{ \frac{\cos\phi + (1 - \nu_1)\sin\phi \tan\phi}{4\sqrt{\pi}\cosh(\pi\varepsilon) \left(\Sigma_{r\theta}^I(\theta)\cos\psi' + \Sigma_{r\theta}^{II}(\theta)\sin\psi'\right)} \right\}^2. \tag{2}$$

Here r_c is the dislocation core cutoff in the metal, μ_I is the shear modulus and ν_I the Poisson ratio of the metal, α is the Dundurs parameter which characterizes the elastic combination of the bimaterial, θ is the inclination angle of the slip plane with respect to the crack plane, ϕ is the angle between the Burgers vector and the normal to the crack front, $\Sigma_{r\theta}^I(\theta)$ are the angular functions given in [3], which correspond to traction across the interface at θ =0 of tensile and in-plane shear, respectively. Equation (2) reveals that G_{disl} is a strong function of the inclination angle θ and the local phase angle ψ' .

Unlike the typical situation when the local phase angle is defined based on a "laboratory" length scale, the distinction between ψ and ψ in this context becomes important because the oscillatory stress field can give rise to a significant shift in the ratio of mode II to mode I type conditions when considering atomic-scale distances from the crack tip. For the Cu/sapphire

specimen shown in Fig. 2 under four-point bending conditions the loading phase angle ψ is about -52°, while the local phase angle ψ is about -79°, indicating a significant mode II component of loading. Under these conditions, equation (2) gives the G_{disl} against θ as plotted in Fig. 5. The model predicts that G_{disl} is about 0.86 J/m² for cracking in the [114]Cu direction and (111) planes with the inclination angle of 125.3° are potentially active; the (111) planes with the inclination angle of 54.7° are inactive because an extremely high value of G_{disl} is needed for dislocation nucleation on these planes. For the cracking direction of [114]Cu, G_{disl} is predicted to be 4.9 J/m² and the potentially active slip planes are (111) which inclined at 164.2°; the (111) planes, in this case the inclination angle is 15.8°, are inactive. The parameter G_{cleav} , a measure of the coherence of the interface, is assumed to be independent of the cracking direction. As a reference, a lower bound of 0.475 J/m² might be quoted from a measurement of the adhesion of the Cu/Al₂O₃ interface [7]. Hence, dislocation emission is favored in the $[114]_{Cu}$ direction and brittle crack growth should be favored in the $[114]_{Cu}$ direction, a prediction supported by our experimental results.

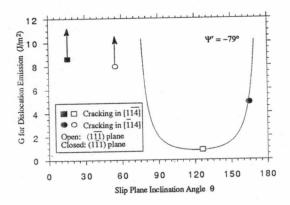


Fig. 5. The energy release rate for dislocation emission, G_{disl} , as a function of the inclination angle, θ , for the Cu/sapphire specimen under four-point bending conditions.

As a comparison, we quote here the calculations of the Peierls-approach by Beltz and Rice [5], which give G_{disl} =0.505 J/m² for the ductile direction and G_{disl} =2.76 J/m² for the brittle direction. There is a factor of 6 difference in G_{disl} for crack growth in the opposite directions and indeed, dislocation emission is preferred in the [114]_{Cu} direction and decohesion occurs in the [114]_{Cu} direction as our experiments showed.

It is interesting to note that the ductile direction in Wang and Anderson's Cu bicrystals under tension conditions is the brittle direction in our Cu/sapphire specimens under bending conditions and vice versa, a result also predicted by Rice et.al [3]. This is attributable entirely to the phase angle effect and is discussed in more detail in [8].

CONCLUSIONS

The ductile versus brittle response of a stressed interfacial crack is not only interface structure dependent, but also direction dependent. An interfacial crack, which propagates in a brittle manner in one direction, might be ductile in the opposite direction. The different fracture behavior of bimaterial interfaces may be understood, at least qualitatively, by comparing the

crack tip energy release rate for dislocation emission from the crack tip against that for cleavage decohesion of the interface. The local phase angle exercises a strong influence upon the ductile versus brittle response of an interfacial crack.

Acknowledgements: We are grateful to J.R. Rice for helpful discussions. This work is supported by NSF through the MRL at Harvard University (grant DMR-89-20490) and a University Research Initiative, through an ONR/DARPA contract at UCSB (subcontract POAVB38639-0).

References

- [1]. P.M. Anderson and J.R. Rice, Scripta Metall. 20, 1467 (1986) and P.M. Anderson, Ph.D. thesis, Harvard University, Cambridge, Mass. (1986).
- [2]. J.-S. Wang and P.M. Anderson, Acta metall. mater. 39, 779 (1991).
- [3]. J.R. Rice, Z. Suo and J.-S. Wang, in Metal-Ceramic Interfaces, Acta-Scripta Metallurgical Proceedings Series, Vol. 4, edited by M. Rühle, A.G. Evans, M. F. Ashby, and J.P. Hirth, pp. 269-294, Pergamon Press, Oxford (1990).
- [4]. J. R. Rice and R. Thomson, Phil. Mag., 29, 73(1974).
- [5]. J. R. Rice, "Dislocation Nucleation from a rack Tip: An Analysis Bases on the Peierls Concept", J. Mech. Phys. Solids, 1991, in press.

 [6]. G.E. Beltz and J.R. Rice, "Dislocation Nucleation at Metal/Ceramic Interfaces", submitted
- to Acta metall. mater., 1991.
- [7]. M. Nicholas, J. Mat. Sci., 3, 571(1968).
- [8]. G.E. Beltz and J.-S. Wang, "Crack Direction Effects along Copper/Sapphire Interfaces", Submitted to Acta metall. mater., 1991.