The influence of surface stress on dislocation emission from sharp and blunt cracks in f.c.c. metals

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Abstract

We use computer simulations to study the behavior of atomically sharp and blunted cracks in various f.c.c. metals. The simulations use effective medium potentials which contain many-body interactions. We find that when using potentials representing platinum and gold a sharp crack is stable with respect to the emission of a dislocation from the crack tip, whereas for all other metals studied the sharp crack is unstable. This result cannot be explained by existing criteria for the intrinsic ductile/brittle behavior of crack tips, but is probably caused by surface stresses. When the crack is no longer atomically sharp dislocation emission becomes easier in all the studied metals. The effect is relatively strong; the critical stress intensity factor for emission to occur is reduced by up to 20%. This behavior appears to be caused by the surface stress near the crack tip. The surface stress is a consequence of the many-body nature of the interatomic interactions. The enhanced dislocation emission can cause an order-of-magnitude increase in the fracture toughness of certain materials, in which a sharp crack would propagate by cleavage. Collisions with already existing dislocations will blunt the crack, if this prevents further propagation of the crack the toughness of the material is dramatically increased.

§1. Introduction

One of the major problems in modeling fracture in materials is the enormous range of length-scales that enter the problem (Carlsson and Thomson 1998). The atomic processes near the crack tip require atomic-scale modeling, but the long-range elastic field of a crack tip may interact with dislocations and dislocation sources too far from the crack tip to allow treatment with atomic-scale methods, except for a few highly idealized configurations. More direct interactions between crack tips and dislocations have also been suggested, including the proposal that collisions between the crack tip and dislocations may both be likely and be important for the fracture toughness of real materials (Mesarovic 1997). Here we concentrate on the atomic-scale behavior of the crack tip, especially in the context of this proposal.

The main conclusion of Mesarovic's work is that the elastic field of a moving crack will attract preexisting dislocations towards the crack, causing them to collide with the crack or at least to pass so close to the crack that an oppositely signed dislocations will be emitted. This will usually cause local blunting of the crack front. Mesarovic assumes that blunting a segment of the crack front causes that segment to arrest, forcing the remainder of the crack to move around the arrested crack. This causes the *local* crack tip toughness (Γ_{tip}) to be increased significantly. A positive feedback mechanism then ensues. The increased crack tip toughness causes a larger stress in the surrounding material, increasing the activity of the dislocations and dislocation sources, thus further raising the fracture toughness by a dramatic increase in the shielding of the crack (Beltz, Rice, Shih and Xia 1996; Mesarovic 1997).

This model clearly depends on the ability of a single dislocation to arrest the crack by blunting it. It thus becomes important to understand how crack blunting affects the intrinsic behavior of the crack tip. By analogy to the stress field near an elliptic crack, it is generally assumed that blunting a crack will dramatically reduce the stress concentration at the crack tip, and thus make both crack propagation and dislocation emission much harder even after a single layer of blunting (Paskin, Massoumzadeh, Shukla, Sieradzki and Dienes 1985; Gumbsch 1995). In a previous paper (Schiøtz, Canel and Carlsson 1997) we found that not to be the case. We studied the effect of blunting on subsequent dislocation emission or cleavage for a crack in a two-dimensional hexagonal lattice, with the interatomic interactions described by a simple pair potential. We reached two main conclusions: First, the effects of the crack blunting on the elastic fields around the crack are minimal, even at very short ranges. This is because the singularity of a 60° wedge crack is almost as strong as for a sharp crack (the power is -0.488 compared to -0.5). Secondly, the non-linearities in the interatomic interactions cause the blunting to have some effect: a slight increase in the stress intensity factor required to cleave, and a tendency to favor emission in stead of cleavage as soon as a single layer of blunting is introduced.

Since these effects are dependent on the interatomic potential used, we decided to perform atomic-scale simulation of crack blunting using more realistic many-body potentials for selected f.c.c. metals (Ni, Cu, Pd, Ag, Pt, Au). These simulations are described in this paper. Rather than attempting an exhaustive set of simulations of all likely crack shapes, we have focussed on a single shape (the shape previously studied), and focus our attention on the effects of including many-body interactions in simulations of this particular shape. As we shall see, the effects we observe will apply for a large class of crack shapes.

We find that the inclusion of many-body effects in the interatomic potential dramatically enhances the effects of crack blunting. This is mainly caused by the introduction of surface stresses, which are absent in models based on a nearest-neighbor pair potential. For most materials surface stresses are tensile[1], and a tensile stress in the surface at the end of a blunt crack will increase the resolved shear stress on

[1] We here use the convention that the surface stress is *tensile* if the surface is under tension, i.e. if the energy of the *surface* atoms could be reduced by reducing the lattice constant. Unfortunately the opposite definition is sometimes also seen.

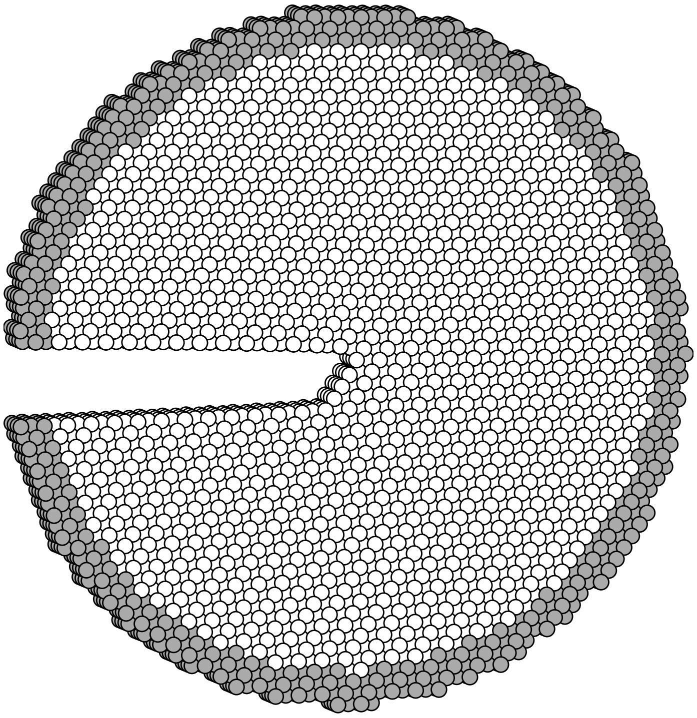

Figure 1: The initial geometry of the simulation cell. The grey atoms are static atoms. Their positions are fixed to match the displacement field of the crack as given by anisotropic linear elasticity (Sih and Liebowitz 1968). The white atoms are dynamic atoms, which are allowed to move. Their positions are energy-minimized for any given elastic load (given by the positions of the static atoms). In the system shown here four layers of blunting are applied to the crack.

a dislocation about to be emitted, thus enhancing dislocation emission. We see reductions of the stress intensity factor required for dislocation emission of up to 20% caused by just a few layers of blunting, this is enough to change the behavior of the crack from brittle crack propagation to dislocation emission.

The simulations also provide an opportunity to test two recently proposed criteria for the intrinsic behavior of sharp cracks (Rice 1992; Zhou, Carlsson, and Thomson 1994). We find that neither of the criteria are able to predict whether sharp cracks in the investigated metals behave in an intrinsically ductile or brittle manner. The deviations seem to be caused by surface stresses in the crack faces. The ductility criterion proposed by Zhou *et al.* may be modified to take this into account.

§2. Computer simulations

We have simulated the emission of the leading partial dislocation from a crack using the geometry shown in figure 1. The simulation cell consists of a cylinder where the atoms near the surface of the cylinder have fixed displacements (static atoms), and the atoms inside the cylinder are free to move (dynamic atoms). Periodic boundary

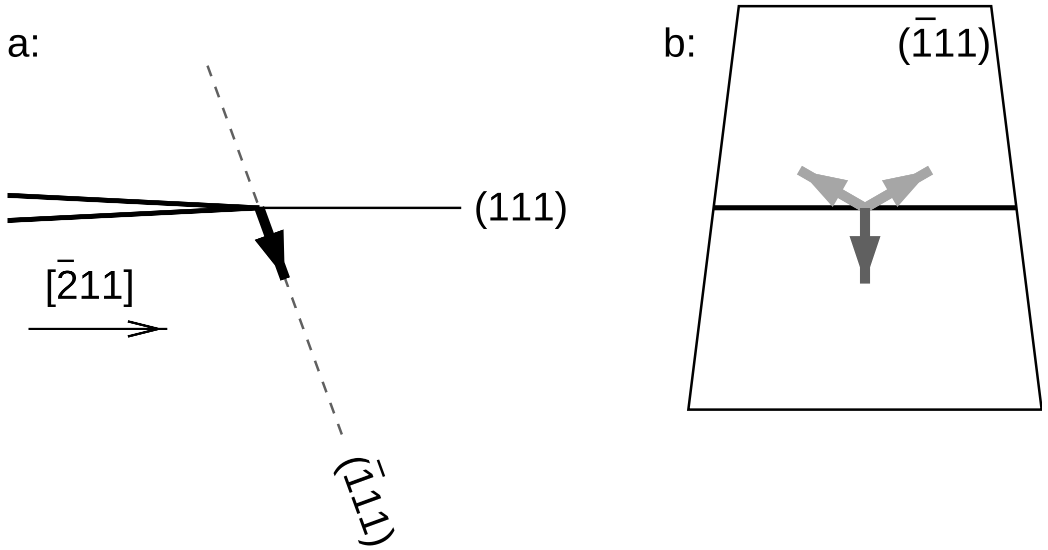

Figure 2: The orientation of the crack. (a) Side view. The crack is moving on the (111) plane in the [$\bar{2}$11] direction. A partial dislocation can be emitted on the ($\bar{1}$11) plane; the thick arrow shows its Burgers vector. The (111) plane is not a mirror plane. Emission in the upward direction would have to happen in the same ($\bar{1}$11) plane, and thus in a "backwards" direction with respect to the crack. (b) Front view of the crack showing the Burgers vectors of the possible partial dislocations. The dislocations that can be emitted upward (lighter grey) have a large screw component in their Burgers vector, and therefore do not couple as strongly to the stress field of the mode I crack.

conditions are applied in the direction along the cylinder axis (the z-axis). We create a sharp crack by first displacing all the atoms according to the displacement field of a crack loaded at the Griffith criterion. We then minimize the energy with respect to all coordinates of the dynamic atoms to investigate if the sharp crack is stable. To create a blunt crack we proceed in a similar fashion. First we remove one to five half-layers of atoms to create the crack. Then we displace all the atoms. The displacement field around a blunt crack is not known analytically, but at large distances compared to the blunting the displacement field will be identical to that of a sharp crack. We therefore use that expression for the field; any error introduced near the crack tip will quickly be removed by the minimization algorithm. We can then gradually step up the loading of the crack, until the leading partial dislocation is emitted or the crack cleaves.

We have chosen a (111)[2$\bar{1}\bar{1}$] orientation of the crack, i.e. the crack moves along a (111) plane in the [$\bar{2}$11] direction. Partial dislocations can be emitted on the ($\bar{1}$11) plane. Since the (111) plane is not a mirror plane there is only one slip plane, but dislocations can be emitted in both directions. Linear elasticity favors emission in the "forward" direction with respect to the crack. The leading partial dislocation emitted in the favored "forward" direction has pure edge character, whereas the leading partial dislocation that could potentially be emitted in the backwards direction has a large

Quantity		Ni	Cu	Pd	Ag	Pt	Au
d	(Å)	3.491	3.592	3.878	4.063	3.921	4.055
C_{11}	(GPa)	242.9	172.8	217.6	125.7	319.0	196.7
	Experiment:	261.2	176.2	234.1	131.5	—	201.6
C_{12}	(GPa)	150.8	116.0	162.3	87.49	258.9	162.6
	Experiment:	150.8	124.9	176.1	97.3	—	169.7
C_{44}	(GPa)	147.5	90.60	75.42	54.57	80.23	46.77
	Experiment:	131.7	81.8	71.2	51.1	—	45.4
$\gamma_{\mathrm{surf}}^{111}$	(J/m^2)	1.684	1.036	.6677	.5472	.7492	.5143
	ab initio:	2.011	1.952	1.920	1.172	2.299	1.283
$\gamma_{\mathrm{surf}}^{100}$	(J/m^2)	1.800	1.125	.7663	.6145	.8766	.5990
	ab initio:	2.426	2.166	2.326	1.200	2.734	1.627
f^{111}	(J/m^2)	-0.30	0.265	1.104	0.486	1.941	1.291
	ab initio:	—	—	3.685	—	6.761	2.772
f^{100}	(J/m^2)	1.041	1.017	1.328	0.788	1.978	1.327
	ab initio:	—	—	2.211	1.682	5.656	3.140
γ_{sf}	(mJ/m^2)	54	31	6.4	8.2	7.4	8.0
	ab initio:	187	56	225	34	393	59
γ_{us}	(mJ/m^2)	278.2	173.6	147.6	114.2	160.9	100.4
K_G	$(MJm^{-5/2})$	.9825	.6194	.4843	.3612	.5479	.3476
$\gamma_{\mathrm{us}}/\gamma_{\mathrm{surf}}^{111}$		.165	.168	.221	.209	.215	.195
$\gamma_{\mathrm{us}}/\mu b$		.0182	.0180	.0166	.0170	.0167	.0174
$\frac{\gamma_{\mathrm{us}}}{\mu b}\left(1+\frac{f^{111}}{3\gamma_{\mathrm{surf}}^{100}}\right)$		.0172	.0194	.0246	.0215	.0290	.0299

Table 1: Elastic constants, surface- and planar fault energies for six f.c.c metals in the Effective Medium Theory. d is the lattice constant, C_{11}, C_{12} and C_{44} are the elastic constants. $\gamma_{\mathrm{surf}}^{111}$ and $\gamma_{\mathrm{surf}}^{100}$ are the surface energies of the (111) and (100) surfaces. f^{111} and f^{100} are the surface stresses. γ_{sf} and γ_{us} are the stacking fault energy and the unstable stacking energy. K_G is the Griffith critical stress intensity factor in plane strain for the crack orientation under consideration, calculated from $\gamma_{\mathrm{surf}}^{111}$ and the elastic constants. Experimental values: elastic constants are from Kittel (1996). *Ab initio* calculations: γ_{surf} from Vitos, Ruban, Skriver and Kollár; f^{111} for Pt and Pd from Feibelman (1995), Au(111) from Needs and Mansfield (1989); f^{100} from Fiorentini, Methfessel and Scheffler (1993); γ_{sf} from Rosengaard and Skriver (1993).

screw component, and therefore couples less strongly to the stress field under mode I (pure opening) loading. See Figure 2. If the crack direction were reversed (i.e. $[2\bar{1}\bar{1}]$ instead of $[\bar{2}11]$) the situation would be reversed, and the system would have the choice between emitting an unfavorable screw-like dislocation in the favorable forward dislocation, or a favorable dislocation in an unfavorable direction. This would lead to a suppression of the emission and a more brittle behavior.

The interatomic interactions are described by the Effective Medium Theory (Ja-

Blunting	Ni	Cu	Pd	Ag	Pt	Au
			Cleavage of sharp crack:			
0	*unstable*	*unstable*	*unstable*	*unstable*	0.98–1.07	0.98–1.05
			Emission from blunt crack:			
1	0.85	0.87	1.01	0.94	1.05	1.03
2	0.80	0.80	0.86	0.83	0.86	0.83
3	0.80	0.78	0.82	0.81	0.82	0.79
4	0.81	0.79	0.82	0.82	0.81	0.77
5	0.82	0.80	0.82	0.83	0.81	0.78

Table 2: Critical load as a function of crack blunting, given in units of the Griffith load (K_G). First line (blunting = 0): The interval where the sharp crack is stable. For loads above the given interval the crack advances, below it it retreats. For some metals a sharp crack is unstable and spontaneously emits a dislocation. The following lines (blunting > 0): The load at which the leading partial dislocation is emitted.

cobsen, Nørskov and Puska 1987; Jacobsen, Stoltze and Nørskov 1996). The main materials parameters for the simulated materials are given in table 1. All values calculated are given for the equilibrium lattice constants of the EMT-metals. The equilibrium lattice constants differ *slightly* from the values used to construct the original EMT parameters, since the extension of the interactions beyond nearest neighbors (Stoltze 1990; Jacobsen *et al.* 1996) causes a contraction of the lattice of around 0.5%. It is seen that the elastic constants are close to the experimental values, but that the surface energies and stresses are quite low.

The surface stresses presented in table 1 were calculated from the difference in the energy variation versus strain of a slab and a bulk system. Care was taken to ensure convergence with respect to system size. As a test, the surface stresses were also calculated using an atomic-level definition of the stress tensor (Egami, Maeda and Vitek 1980; Ray and Rahman 1984). The two calculations agree.

§3. Results

The results of the simulations are shown in table 2. There are two main results. First, the simulations of the sharp crack show that the investigated FCC metals fall in two groups: platinum and gold are intrinsically brittle (a sharp crack is stable, and will propagate), whereas nickel, copper, palladium and silver are intrinsically ductile (a sharp crack is unstable, and will emit a dislocation). See Figure 3. We find a small amount of lattice trapping for platinum and gold, approximately 5%. We see from the simulations that palladium and silver are very close to the transition between intrinsically brittle and ductile behavior. For these two metals a sharp crack loaded at the Griffith load will remain stable, but when the load is increased the crack will emit a dislocation before the lattice trapping is overcome.

The second main result is the behavior of the blunt crack. Here all six metals behave in a similar way. After just one layer of blunting the crack will no longer

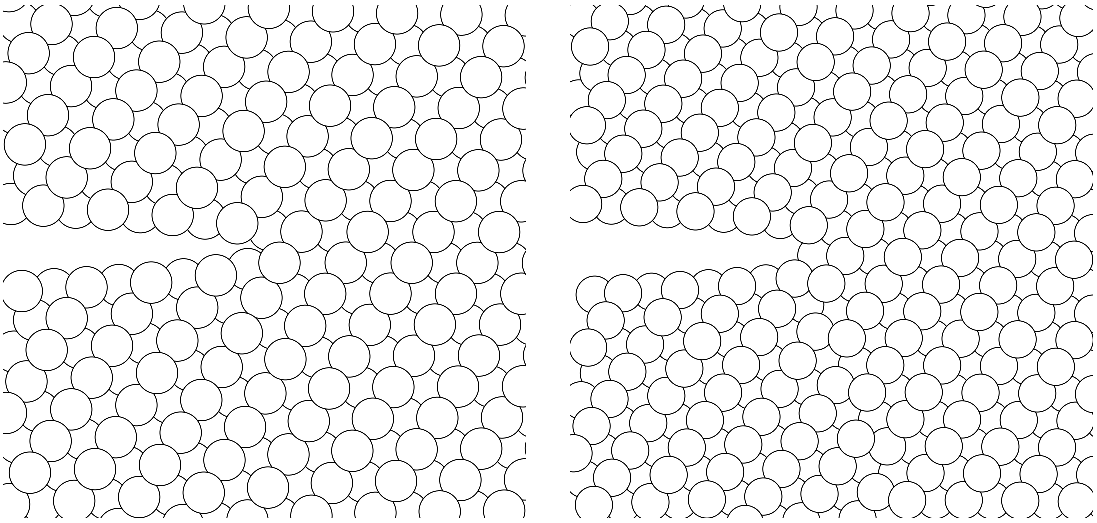

Figure 3: The behavior of sharp cracks. *Left:* A sharp crack in gold is stable. No dislocation is emitted. *Right:* A sharp crack in nickel is unstable. A partial dislocation is emitted (down and to the right).

cleave, but emits a dislocation. Further blunting of the crack seems to favor the emission further, at least until the crack is blunted by three layers. Increasing the blunting beyond three layers has no or little effect on the emission. For the largest amount of blunting investigated (four and five layers of blunting) we find a slight reversal of the effect - increasing the blunting seems to increase the load required to emit a dislocation a little. The total reduction of the load required to emit a dislocation is around 20% compared to the Griffith load.

§4. Discussion

The results presented in the previous section show both major similarities to and differences from our previously published results for blunt cracks in a two-dimensional lattice (Schiøtz *et al.* 1997). The main similarity is the change in behavior of the crack for some force law parameters, a change from brittle behavior of the sharp crack to ductile behavior of the blunt crack. The main difference is the ease with which the dislocations are emitted from the blunt crack. In the previous work we saw an *increase* in the critical load when the blunting was increased, even when the crack began emitting dislocations. The emission was thus more a result of inhibiting further cleavage than of enhancing the emission. In this work we instead see a clear *decrease* of the critical load. We further see that this decrease continues until the crack has been blunted by three atomic layers. This behavior is opposite from what one would expect from simple arguments based on linear elasticity, since increased blunting should decrease the stresses near the crack tip, and thus increase the critical loads. We should, however, remember that for a blunt crack with sharp corners this *linear elastic* effect is very small (Schiøtz *et al.* 1997).

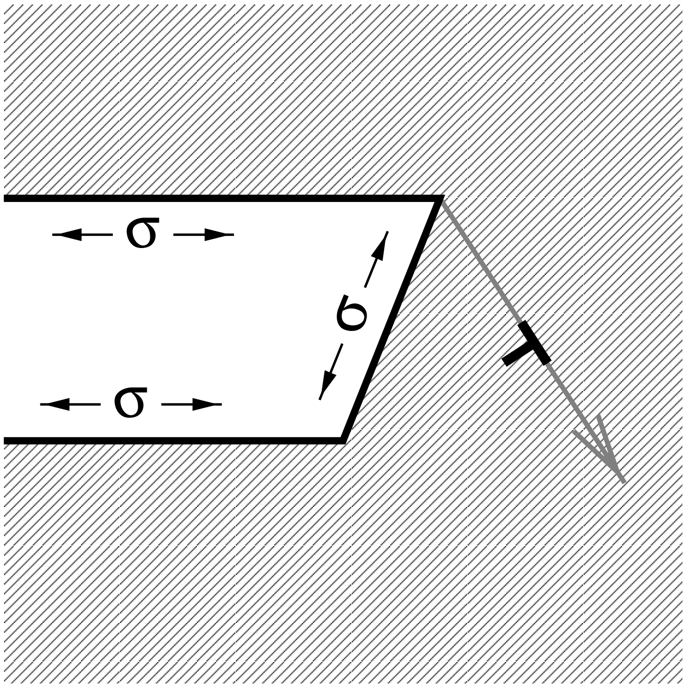

Figure 4: Surface stresses near the tip of a blunt crack. Tensile surface stress in the end surface of the crack will tend to favor dislocation emission on the slip plane shown.

We find that the most probable cause of this difference is the presence of surface stresses in these simulations. The previous work was done using nearest-neighbor pair potentials to describe the interactions between the atoms; in such a potential no surface stress appears. The effective medium theory contains many-body interactions in the potential, and gives a more realistic description of the metal properties. Surface stresses are present in the effective medium theory. As the crack is blunted, a new surface appears at the crack tip, and a surface stress will be present at the new surface.

For all the materials investigated here the surface stress of the created (100) facet is tensile. This stress will naturally change the stress distribution in the system near the crack tip. Most importantly, the tensile stress in the surface at the end of the crack (see figure 4) will cause a resolved shear stress in the plane of an emitted dislocation that favors emission. This is best seen by considering what emission of a dislocation will do to the end surface under tensile stress. As the dislocation is emitted the end surface is enlarged by one row of atoms. This allows the atoms to contract, releasing some of the tensile surface stress. This energy argument is not limited to the geometry studied here. In most geometries of a blunt crack, there will be an "end surface" which will become larger when a blunting dislocation is emitted (see figure 5). A tensile surface stress will thus be partially relieved by the emission of a dislocation, and the surface stress must therefore aid the emission.

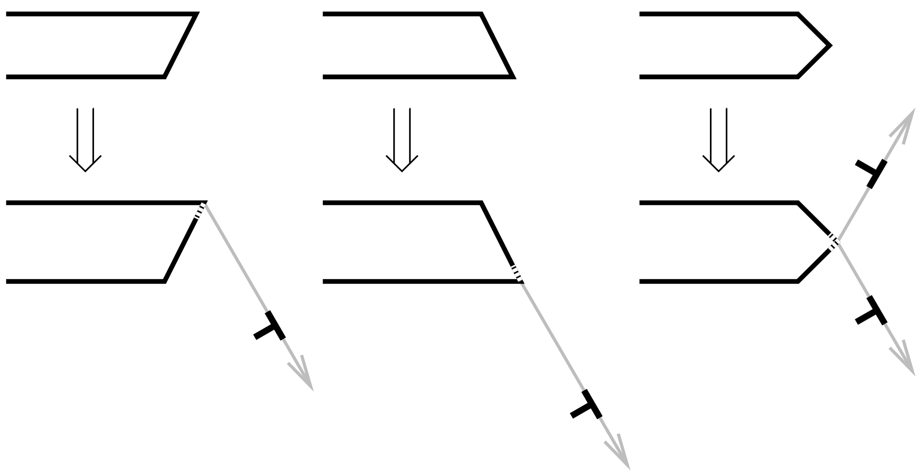

Figure 5: Dislocation emission from various hypothetical crack geometries. In all cases the area of the "end surface(s)" of the crack is increased as a blunting dislocation is emitted. A tensile surface stress will thus be relieved by the dislocation emission: the surface stress will facilitate dislocation emission.

As the size of the end ledge increases, the tensile stress builds up[2] and dislocation emission becomes easier. Once the end surface is sufficiently developed, the surface stress reaches its "macroscopic" value, and further increase of the crack blunting does not increase the surface stress. No further enhancement of the dislocation emission is then seen. For this reason, the critical load is approximately constant when the crack blunting is changed from three to five layers (see table 2). It should be noted, that if the surface stress is constant, the work done by it will to first order not depend on the size of the end surface, nor by how the strain is distributed along it.

To test this hypothesis we compare the shear stress induced by the surface stress to the calculated reduction in the critical load required to emit a dislocation. An order of magnitude estimate of the shear stress induced by the surface stress is f^{100}/d, i.e. the surface stress is distributed over a layer of thickness comparable to the lattice spacing. The influence of this surface stress will then depend on the ratio between this induced shear stress and the shear stress originating from the loading of the crack. The linear elastic expression for the shear stress near a sharp crack loaded in mode I is (Thomson 1986):

$$\sigma_{r\theta} = K_I (2\pi r)^{-1/2} \sin(\theta/2) \cos^2(\theta/2) \tag{1}$$

This describes the stress field around a sharp crack. The θ dependence will change somewhat near a blunt crack, but as already mentioned the r dependence will be es-

[2]The surface atoms are lacking some of their neighbors compared to bulk atoms, the local electron density is thus lower. To compensate for this, it is energetically favorable to reduce the lattice spacing locally. This is a slightly simplified picture of the main cause of the tensile surface stress. When the "new" surface at the end of the crack is small, i.e. when the blunting is low, the atoms will not lack all their neighbors, and the surface stress is expected to be lower.

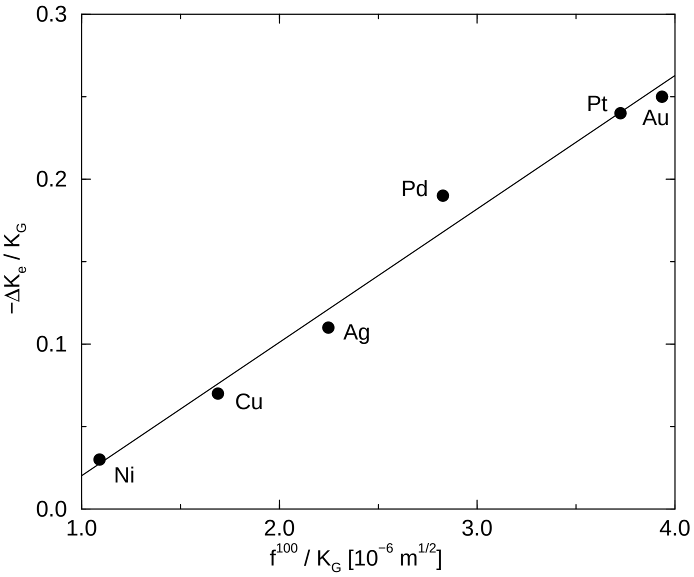

Figure 6: Comparison of the strength of the surface stress and the effect of blunting on the dislocation emission. Along the x-axis is plotted the ratio between the surface stress (f^{100}) and the applied stress measured by the stress intensity factor (K). Along the y-axis is plotted the enhancement of the dislocation emission as given by the change (ΔK_e) in the load required to emit a dislocation measured in units of the Griffith stress.

sentially unchanged. The linear elastic expression is only valid down to r comparable to the interatomic spacing, and at such distances it is only a rough approximation. Since we do not worry about factors of order unity, we will nevertheless use Eq. (1) at $r = d$ (the lattice constant) as a rough estimate of the order of magnitude of the shear stress induced near the crack tip by the loading of the crack. For all the materials considered in this paper, the two estimates are of the same order of magnitude (the ratio varying between 0.4 and 1.3). It is thus plausible that the surface stress may have a significant effect on the dislocation emission.

If the enhanced dislocation emission is indeed a result of the surface stress, its magnitude should be roughly proportional to the surface stress. As a measure of the effect of the blunting we use the relative change of the critical load to emit a dislocation as we change the blunting from one to five layers ($\Delta K_e/K_G$). In Figure 6 we investigate the correlation between the reduction of the critical load ($-\Delta K_e/K_G$), and the ratio between the surface stress (f^{100}) and the applied stress as measured by the critical stress intensity factor (K_G). The remarkably good correlation is a strong support for the hypothesis that the surface stress causes the enhanced dislocation emission.

Since a tensile surface stress will be present in most metals, this mechanism is possible in any metal where the sharp crack behaves in an intrinsically brittle manner, but where the system is not too far from dislocation emission. In these materials collisions between a propagating crack and preexisting dislocations may cause the crack

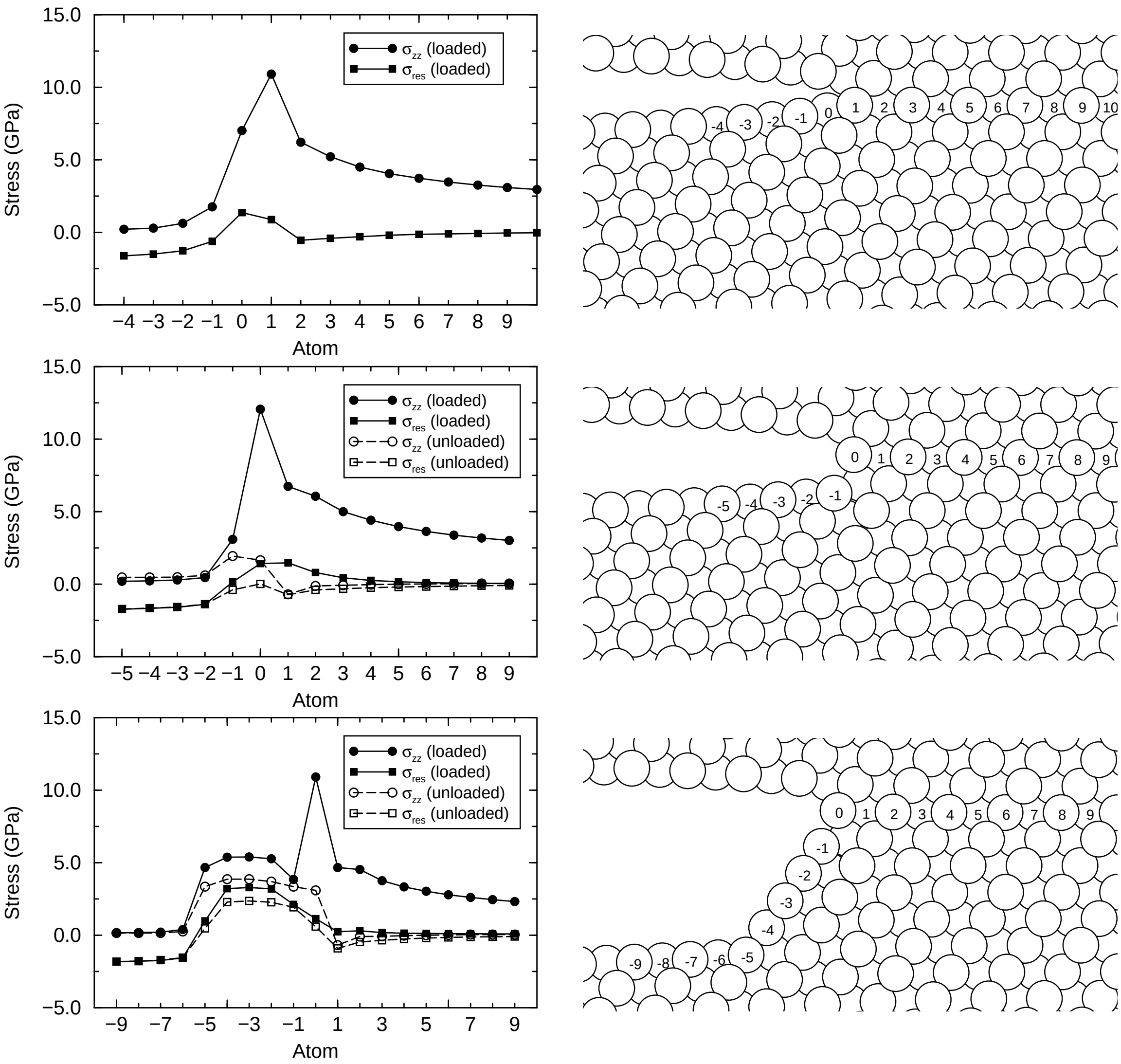

Figure 7: Local stresses at the atoms near the crack tip in gold. The sharp crack is loaded at the Griffith load, the blunt cracks are loaded just below the load required to emit a dislocation. Filled circles show σ_{zz}, i.e. the component of the stress that drives the crack forward. Filled squares show σ_{res} (the resolved shear stress on the dislocation glide plane), i.e. the component of the stress driving dislocation emission. Open symbols show the same quantities, but with no external load on the crack, so that the stresses shown are caused by the surfaces. The sharp crack closes when not loaded, so no open symbols are shown in that case.

to locally become emitting, and if the collisions are common enough the macroscopic response of the material may be ductile in spite of the sharp crack tip being stable in principle.

Figure 7 shows the stresses at selected atoms in three different geometries in gold without loading, and loaded just below the level required to emit a dislocation.

The open symbols are the stresses without a load. They give a measure of how much the surface stresses contribute to the stresses driving the crack (σ_{zz}) and to the resolved shear stress on the dislocation glide plane ($\sigma_{\rm res}$). It is seen that in the case of five layers of blunting, the surface stresses contribute significantly to both σ_{zz} and $\sigma_{\rm res}$ of the atoms near the crack tip, but that the relative contribution to $\sigma_{\rm res}$ is larger. This causes the surface stress to enhance the dislocation emission more than the crack propagation. It should also be noted that *local* stresses near the crack tip may help overcome barriers to crack propagation (lattice trapping), but can not help propagating the crack, as crack propagation is energetically forbidden below the Griffith loading.

Atomic-scale stresses such as those plotted in Figure 7 should be viewed with some scepticism, as there is no unique definition of the atomic-level stress. Although the different definitions give the same answer when averaged over a small region of space, significant differences can be seen in the values for individual atoms (Cheung and Yip 1991).

It has previously been suggested (Thomson, Chuang and Lin 1986; Sieradzki and Cammarata 1994; Cammarata and Sieradzki 1996) that surface stresses may influence dislocation emission from *sharp* cracks. However, the surface stress effect discussed here is of a different nature. In the case of a sharp crack the suggested effect of a tensile surface stress would be to inhibit the emission of dislocations, whereas the tensile surface stress here is seen to *enhance* dislocation emission from blunt cracks.

Gumbsch (1995) has studied sharp and blunt cracks in Ni using the Embedded Atom Method (EAM), a many-body potential very similar to EMT. Surprisingly, he finds that the sharp crack with the $(111)[2\bar{1}\bar{1}]$ orientation studied here is stable, and propagates by cleavage, although other orientations favor dislocation emission. The blunt crack is studied only in the (100)[010] and (100)[011] orientations. In the first case emission of the usual $\frac{a}{6}\langle 211\rangle$ Shockley partial dislocations is geometrically impossible, and the crack is brittle at all levels of blunting. The (100)[011] crack *can* emit partial dislocations, this is seen but only at five layers of blunting, and at a stress significantly above the Griffith stress (1.17 K_G). The different behavior in this work may be due to a different crack tip geometry, since Gumbsch chose a symmetrical configuration, or it may be due to different surface stresses when the EAM potential is used.

The result that some of these f.c.c. metals (Au, Pt) are intrinsically brittle, and some (Ag, Pd) are close to being intrinsically brittle, is surprising in light of the "$\gamma_{\rm us}$" criterion for brittle/ductile behavior proposed by Rice (1992). According to that criterion a crack will be intrinsically ductile if

$$\frac{\gamma_{\rm us}}{\gamma_{\rm surf}} < \frac{2}{Y} \tag{2}$$

where $\gamma_{\rm us}$ is the "unstable stacking energy" (Rice 1992), $\gamma_{\rm surf}$ is the surface energy and Y is a geometrical factor. In our geometry $2/Y$ is approximately 0.30. $\gamma_{\rm us}/\gamma_{\rm surf}$ is listed in table 1 for all the metals studied. It is seen that by this criterion all the metals should be intrinsically ductile, and far from the transition to brittle behavior. It has been suggested that the stress fields near the crack tip changes $\gamma_{\rm us}$ locally.

However this change would result in a lower value of $\gamma_{\rm us}$ and thus in enhanced ductility (Sun, Beltz and Rice 1993). A similar reduction was found by Cleri, Yip, Wolf and Phillpot (1997), who used atomic-scale simulations to calculate the relevant γ describing the barrier for dislocation emission, and found that it was approximately $\frac{1}{2}\gamma_{us}$ for the Lennard-Jones solid they studied. We must therefore conclude that the results presented here are in clear violation of the $\gamma_{\rm us}$ criterion.

Such a violation is consistent with previously obtained results for the behavior of cracks loaded in mode I (pure opening) (Zhou *et al.* 1994; Gumbsch and Beltz 1995). Eq. (2) does not consider the energy cost of creating extra surface at the crack end during dislocation emission. When this so called ledge energy is taken into account a different criterion, where dislocation emission is more difficult, is obtained (Zhou *et al.* 1994). The resulting criterion is independent of the surface energy, and depends only on the unstable stacking energy. For a two-dimensional hexagonal lattice they find that a material is ductile if

$$\frac{\gamma_{\rm us}}{\mu b} < 0.012, \tag{3}$$

but the numeric constant may be different in other crystal structures and other crack geometries. We have also evaluated $\gamma_{\rm us}/(\mu b)$ for these materials, see table 1. It is clearly seen that no value of $\gamma_{\rm us}/(\mu b)$ can be found that divides the intrinsically brittle from the intrinsically ductile materials.

As in the case of the blunt cracks, the surface stresses may be important. The two metals that appear brittle in this study, Pt and Ag, are the two metals with the highest tensile surface stress. This high surface stress is also seen experimentally, as the surfaces tend to reconstruct in a way that relieves the surface stress. Even the closed-packed (111) surfaces of Pt and Au reconstruct in a way that increases the density of surface atoms (see e.g. Sandy, Mochrie, Zehner, Grübel, Huang and Gibbs (1993) and references therein).

When a dislocation is emitted from a sharp crack in the geometry shown in Figure 2a, the lower crack surface is stretched and work is done against the surface stress (Sieradzki and Cammarata 1994). This work is not included in equation (3). The effect of including the surface stress can be estimated from the work of Thomson and Carlsson (1994), where they give theoretical arguments for equation (3). They find that the critical value of the crack extension force $\mathcal{G}_{Ie}$ at emission of a dislocation is

$$Y^2 \frac{\mathcal{G}_{Ie}}{\mu' b} = \frac{\gamma_{\rm us}}{\mu' a} + 8\pi \frac{\gamma_{\rm surf}\gamma_{\rm us}}{(\mu' a)^2} \tag{4}$$

where Y is a geometric factor, μ' is an effective shear modulus, b is the Burgers vector and a is the lattice constant. The critical crack extension force for cleavage is $\mathcal{G}_{Ic} = 2\gamma_{\rm surf}$. The first term in equation (4 is the work done to create the dislocation, if it dominates equation (2) becomes the relevant ductility criterion. The second term is the work done to create the ledge, if it dominates equation (3) determines the behavior.

The work done against the surface stress can be included by replacing $\gamma_{\rm surf}$ in equation (4) by $\gamma_{\rm surf} + \alpha f$, where α is the ratio between how much the crack surface is stretched (u_{tip}) and the width of the created ledge. The work done does not depend on how the strain is distributed:

$$W_{\mathrm{stress}} = \int_{-\infty}^{0} dx\, f\varepsilon(x) = \int_{-\infty}^{0} dx\, f\frac{\partial u}{\partial x} = \int_{0}^{u_{\mathrm{tip}}} du\, f = u_{\mathrm{tip}} f \tag{5}$$

The transition between ductile and brittle behavior happens for $\mathcal{G}_{Ie} = \mathcal{G}_{Ic}$. Neglecting the first term in equation (4) we get a modified criterion for ductility:

$$\frac{\gamma_{\mathrm{us}}}{\mu b}\left(1 + \alpha\frac{f}{\gamma_{\mathrm{surf}}}\right) < C, \tag{6}$$

where C is a constant. This criterion has been included in table 1, setting $\alpha = \cos 70.5° = 1/3$ (the angle between two $\{111\}$ planes). We see that it is in *qualitative* agreement with the simulations: the largest values are found for the metals with brittle behavior (Au and Pt), somewhat lower values for the metals showing a weak tendensy towards brittleness (Ag and Pd), and lowest for Cu and Ni.

Equation 6 should not be taken as a *quantitative* criterion, as too many assumptions and approximations were involved. For example, the two terms in equation (4) are approximately equal in these simulations, so the criterion should be an intermediate between equations (2) and (6). Some of the work done against the surface stress will be recovered by a contraction of the opposite surface, reducing α (in the case of emission in the crack plane $\alpha = 0$ by symmetry). On the other hand, the cost of creating the ledge will be less than the surface energy times the area, as the atoms in the ledge surface have not lost as many neighbors as in a plane surface. This would increase the relative importance of the surface stress versus the surface energy, i.e. effectively increase α. Although equation 6 is not a quantitative ductility critetion, it still provides a qualitative explanation of the trends observed in the simulations.

It should finally be noticed that the observed intrinsic brittleness could be an artifact of the low surface energies obtained in the Effective Medium Theory's descriptions of metallic bonding, although this may to some extend be compensated by a similar underestimation of the unstable stacking energy. However, the test of the ductility criteria is "self-consistent" in the way that the values for γ_{surf} and γ_{us} are evaluated using the same potential that was used in the simulations. In that way even if the values are not exactly the same as the experimental values, the criteria are still tested reliably. Similar considerations apply to the blunt cracks, as both the surface energies and stresses are underestimated. However, since the ratio between them is approximately correct, the magnitude of the effect of crack blunting should be approximately correct.

§5. Conclusions

We have simulated the emission of infinite straight dislocations from crack tips in Ni, Cu, Pd, Ag, Pt and Au modeled by the Effective Medium Theory. We find that a sharp crack is stable and will propagate in Pt and Au, but is unstable in Ni, Cu, Pd and Ag. Thus, gold and platinum are intrinsically brittle whereas the other metals are intrinsically ductile. This behavior is not explained by two recently proposed criteria for intrinsic crack tip behavior. The deviations appear to be caused by stresses in the crack surfaces.

When the cracks are blunted dislocation emission is seen to occur in all the investigated materials at stresses approximately 20% below the theoretical cleavage stress. We propose that this is caused by a tensile surface stress in the end-surface of the crack generating a local stress field that favors emission. This is supported by a strong correlation between the change in critical load when the crack blunting is increased and the strength of the surface stress relative to the stress from the crack tip. This effect is not expected to depend strongly on the details of the geometry of the crack tip.

A consequence of this enhanced emission is a new possible mechanism for ductile behavior of otherwise intrinsically brittle materials (Mesarovic 1997). In such materials crack blunting, caused e.g. by collisions between the moving crack tip and preexisting dislocations, could arrest the crack and cause it to emit dislocations instead. Such crack arrest has been shown to be able to cause a dramatic increase in the fracture toughness of the material (Beltz *et al.* 1996; Mesarovic 1997).

Since most metals exhibit tensile surface stresses, this mechanism may be active in other intrinsically brittle materials, and may be a cause of increased fracture toughness in a class of materials. Even if the intrinsic brittleness that we observe for gold and platinum turn out to be an artifact of the low surface energies in the Effective Medium Theory, other metals may be intrinsically brittle but be observed to be ductile because the cracks are arrested by collisions with preexisting dislocations.

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