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Ab initio calculation of tensile strength in iron

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ABSTRACT

A tensile test in ferromagnetic iron for loading in [001] and [111] directions is simulated by *ab initio* electronic structure calculations using all-electron full-potential linearized augmented-plane-wave method within the generalized gradient approximation. The theoretical tensile strengths and Young's moduli of ferromagnetic iron are determined and compared with those of other materials. The magnetic and elastic behaviours of iron under uniaxial tensile loading are discussed in detail and compared with the results for isotropic tension (i.e. for negative hydrostatic pressure). Marked anisotropy of theoretical tensile strength in [001] and [111] direction is explained in terms of higher-symmetry structures present or absent along the deformation paths.

§1. INTRODUCTION

The strength of materials is usually controlled by nucleation and motion of dislocations or microcracks. If such defects were not present, the material loaded in tension would only fail if the theoretical or ideal tensile strength were reached. The stress at which this is achieved is comparable with Young's modulus of the material and it is an upper limit of stresses attainable prior to failure. Until recently loads of this magnitude were approached in studies of the mechanical behaviour of whiskers of very pure metals and semiconductors (Brenner 1956, 1957, Coleman *et al*. 1957, Pearson *et al*. 1957, Nadgorny 1962). However, the ideal strength appears to control both the onset of fracture and the dislocation nucleation in defect-free thin films and, in particular, in nanostructured materials that are currently being developed. This has been confirmed most eloquently by nanoindentation experiments (for example Vinci and Vlassak (1996), Bahr *et al*. (1998), Gouldstone *et al*. (2000), Woodcock and Bahr (2000) and de la Fuente *et al*. (2002)), which suggest that the onset of yielding on the nanoscale is controlled by homogeneous nucleation of dislocations in the small volume under the nanoindenter where stresses approach the theoretical strength. This volume is almost always dislocation free since in well-annealed

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samples the average dislocation spacing is about 1 μm, while the contact area as well as the depth in which large stresses are attained are of the order of 100 nm.

Theoretically, the ideal strength was studied in the past using semiempirical approaches when describing atomic interactions (for a review see for example Milstein and Chantasiriwan (1998) and references therein; ideal shear strengths calculated for all basic cubic structures may be found in the work by Šandera and Pokluda (1993)). However, within such schemes, parameters are fitted to equilibrium properties of the material studied and their transferability to the state when this material is loaded close to its theoretical strength is not warranted. In contrast, *ab initio* electronic structure calculations can be performed reliably for variously strained structures and are thus capable of determining the ideal strength of materials without resort to doubtful extrapolations. Indeed, recently determination of theoretical strength became possible using *ab initio* electronic structure methods based on the density functional theory. Such calculations of theoretical tensile strength have been made for copper (Esposito *et al.* 1980, Šob *et al.* 1998a), TiC (Price *et al.* 1992), tungsten (Šob *et al.* 1997a, Roundy *et al.* 2001), NiAl (Šob *et al.* 1998a,b), aluminium (Li and Wang 1998, Kitagawa and Ogata 1999, Ogata and Kitagawa 1999), β-SiC (Li and Wang 1999), AlN (Kitagawa and Ogata 1999, Ogata and Kitagawa 1999), and recently also for $MoSi_2$ and WSi_2 (Friák *et al.* 2001a, 2003), diamond (Telling *et al.* 2000, Roundy and Cohen 2001), silicon and germanium (Roundy and Cohen 2001), molybdenum and niobium (Luo *et al.* 2002), iron (Friák *et al.* 2001b, Clatterbuck *et al.* 2002) and Si_3N_4 (Ogata *et al.* 2001, 2003, Kocer *et al.* 2003).

The aim of the present contribution is to perform an *ab initio* study of elastic, magnetic and structural behaviour of iron under uniaxial loading in the [001] and [111] directions, to determine the value of theoretical tensile strength and to compare the results with those for hydrostatic tension.

§ 2. Method and computational details

To simulate a tensile test, we first calculate the total energy of the material in the ground state. Then, in the second step, we apply some elongation of the crystal along the loading axis by a fixed amount ε that is equivalent to the application of a certain tensile stress σ. For each ε, we minimize the total energy, relaxing the stresses $\sigma_{\perp 1} = \sigma_{\perp 2}$ in the directions perpendicular to the loading axis. The stress σ is given by (Rasky and Milstein 1986)

$$\sigma = \frac{c}{V}\frac{\partial E}{\partial c} = \frac{1}{Ac_0}\frac{\partial E}{\partial \varepsilon}, \tag{1}$$

where E is the total energy per repeat cell, V is the volume of the repeat cell, c is the dimension of the repeat cell in the direction of the loading, $A = V/c$ is the area of the basis of the repeat cell in the plane perpendicular to the loading axis and c_0 is the value of c in the underformed state. The inflection point in the total energy versus ε dependence yields the maximum attainable tensile stress; if no other instability (violation of some stability condition, soft phonon modes, magnetic spin arrangement, etc.) occur before reaching the inflection point, it corresponds to the theoretical tensile strength σ_{th}. The bcc structure of iron becomes bct under uniaxial loading along the [001] axis and trigonal under [111] uniaxial loading conditions.

As far as hydrostatic deformation is concerned, iron keeps the bcc structure and the dimensions of the crystal change in all directions homogeneously. The hydrostatic stress σ is then calculated using the formula

$$\sigma = \frac{\partial E}{\partial V}. \tag{2}$$

Our calculations have been performed by means of all-electron full-potential linear augmented-plane-wave method (using the WIEN97 code (Blaha *et al*. 1997), which is an improved and updated UNIX version of the original copyrighted WIEN code (Blaha *et al*. 1990)) within the generalized gradient approximation (Perdew *et al*. 1996). The muffin-tin radius of iron atoms of 1.90 au is kept constant for all calculations, the number of **k** points in the Brillouin zone is equal to 6000, and the product $R_{\mathrm{MT}}k_{\max}$ of the muffin-tin radius and the maximum reciprocal space vector is equal to 10. The maximum ℓ value $\ell_{\max}$ for the waves inside the atomic spheres and the largest magnitude $G_{\max}$ of the reciprocal vector **G** in the charge Fourier expansion are set to 12 and 15 respectively.

§ 3. Results and discussion

The total energy of ferromagnetic iron as a function of elongation ε is shown in figure 1 (*a*) for both [001] and [111] directions of loading and compared with the result for hydrostatic strain (we apply isotropic tension, i.e. negative hydrostatic pressure). The dimensionless parameter ε reflects the changes in the crystal dimension in the direction of loading in the case of tensile test simulations and an increase in the bcc lattice parameter in the case of hydrostatic loading.

Craievich *et al*. (1994) have shown that some energy extrema on constant-volume transformation paths are dictated by the symmetry. That is, most of the structures encountered along the transformation paths between some higher-symmetry structures, say between bcc and fcc at the Bain path, have a symmetry that is lower than cubic. At those points of the transformation path where the symmetry of the structure is higher the derivative of the total energy with respect to the parameter describing the path must be zero. These are the so-called symmetry-dictated extrema. However, other extrema may occur that are not dictated by symmetry and reflect properties of the specific material. The same is true for the transformation paths corresponding to uniaxial loading (Milsten and Farber 1980, Alippi *et al*. 1997). Configurations corresponding to energy minima at the transformation paths represent stable or metastable structures and may mimic atomic arrangements that could be encountered when investigating thin films (Alippi *et al*. 1997) and extended defects such as interfaces and dislocations (Šob *et al*. 1997b, Paidar *et al*. 1999).

In contrast with the tetragonal deformation path, the trigonal deformation path (for loading along the [111] axis) passes from the bcc ground-state structure to the simple cubic (sc) structure exhibiting at this point a maximum of the total energy (Šob *et al*. 1997a,b). The symmetry-dictated energy extrema are easily visible in figure 1 (*a*), namely the ground-state minimum at the bcc structure and the maximum at the fcc (tetragonal) and sc (trigonal) deformation path.

The total energy dependences have a parabolic convex character in the neighbourhood of the symmetry-dictated minimum in the bcc structure (ground state). With increasing value of ε the curves reach (owing to the nonlinear effects) their

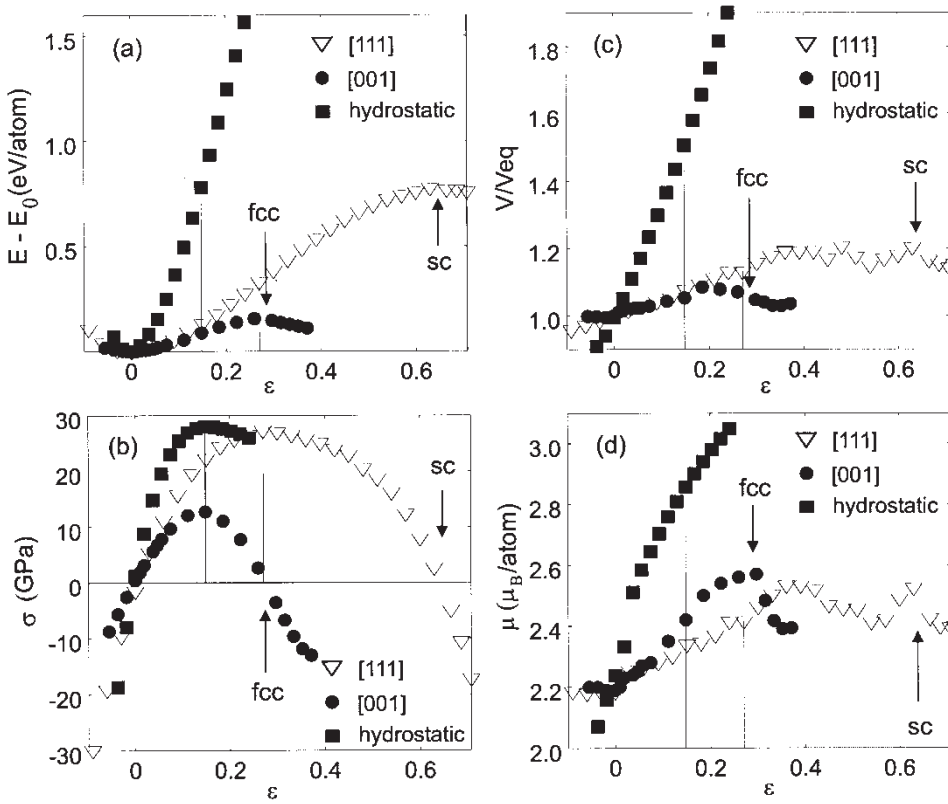

Figure 1. (*a*) Total energy per atom relative to the energy of the equilibrium state, (*b*) stress, (*c*) relative atomic volume ratio with respect to the equilibrium volume V_{eq} and (*d*) magnetic moment per atom of ferromagnetic iron loaded hydrostatically (■) and uniaxially along the [001] (●) and [111] directions (▽) versus elongation ε. The relative elongation ε reflects the changes in the a_{bcc} lattice parameter for hydrostatic loading and in the case of uniaxial tensile test simulations the increase or decrease of the crystal dimension in the direction of loading. The vertical thin lines show the states exhibiting maximum stress (i.e. the theoretical tensile strength). Incidentally, the maximum stresses for [001] uniaxial loading and that for hydrostatic loading are reached at nearly the same strain ε and, therefore, the corresponding vertical lines coincide.

inflection points (indicated by vertical lines in figure 1) and become concave. The inflection point for [001] uniaxial loading occurs (most probably incidentally) for nearly the same elongation of $\varepsilon = 0.15$ as for hydrostatic loading. In case of the [001] tensile test simulation, this elongation corresponds to the value of the lattice parameter in the direction of loading equal to 6.20 au (the perpendicular dimensions are relaxed) and, in the case of hydrostatic strain, to the bcc structure with the lattice constant of 6.20 au.

From the total energy dependences shown in figure 1 (*a*), we may directly determine the values of Young's moduli Y for [001] and [111] directions of loading and the bulk modulus B in the equilibrium ground state. Using the values of contraction in the directions perpendicular to the loading axis, we also may calculate the

corresponding Poisson's ratios ν. These quantities may be expressed in terms of the elastic constants c_{ij}:

$$\left(\frac{\Delta E}{V_{\mathrm{eq}}}\right)^{[001]} = \tfrac{1}{2} Y^{[001]} \varepsilon^2_{[001]}, \qquad Y^{[001]} = \frac{(c_{11}-c_{12})(c_{11}+2c_{12})}{c_{11}+c_{12}}, \qquad \nu^{[001]} = \frac{c_{12}}{c_{11}+c_{12}}, \tag{3}$$

$$\left(\frac{\Delta E}{V_{\mathrm{eq}}}\right)^{[111]} = \tfrac{1}{2} Y^{[111]} \varepsilon^2_{[111]}, \qquad Y^{[111]} = 3\frac{c_{44}(c_{11}+2c_{12})}{c_{44}+c_{11}+2c_{12}}, \qquad \nu^{[111]} = \frac{c_{11}+2c_{12}-2c_{44}}{2(c_{11}+2c_{12}+c_{44})}, \tag{4}$$

$$B = V_{\mathrm{eq}} \left.\frac{\partial^2 E}{\partial V^2}\right|_{V=V_{\mathrm{eq}}} = \frac{c_{11}+2c_{12}}{3}. \tag{5}$$

Here ΔE is the change of the total energy per atom and V_{eq} is the equilibrium atomic volume.

Table 1 summarizes the calculated Young's moduli and Poisson's ratios together with available experimental data and the values based on equations (3) and (4) using experimental elastic constants (Simmons and Wang 1971). Our value of bulk modulus, namely 186 GPa, is in very good agreement with experimental value of 172 GPa (Acet *et al.* 1994) (lattice constant extrapolated to $T = 0$ K).

The fact that the theoretical tensile strength in the [111] direction is about twice that in the [001] direction may be explained as follows. The structural energy difference $E_{\mathrm{sc}} - E_{\mathrm{bcc}}$ affecting the shape of the trigonal deformation path is about five times the difference $E_{\mathrm{fcc}} - E_{\mathrm{bcc}}$ that affects the shape of the tetragonal deformation path (755 meV atom^{-1} compared with 155 meV atom^{-1}). Consequently, to reach the nearby maximum for the [111] loading, the total energy must increase much more than for the [001] loading. At the same time, in the former case the increase occurs for larger values of ε than in the latter case since the metastable sc structure, which occurs for [111] loading, is obtained for higher elongation ε than the fcc structure that occurs for [001] loading ($\varepsilon^{[111]}_{\mathrm{th}}/\varepsilon^{[001]}_{\mathrm{th}} = 0.64/0.27 = 2.37$ (see figure 1 (*a*))). As a result, the inflection point at the trigonal deformation path is attained for higher

Table 1. Young's moduli Y and Poisson's ratios ν obtained from uniaxial tensile test simulation along the [001] and [111] directions. The results are compared with available experimental data and also with values based on equations (3) and (4) using experimental elastic constants (Simmons and Wang 1971).

	Y (GPa)	ν
Simulation, [001]	155	0.37
Experimental, [001]	132[a]	—
From c_{ij}, [001]	143	0.36
Simulation, [111]	285	0.23
Experimental, [111]	284[a]	—
From c_{ij}, [111]	296	0.21

[a]Gilman (1963).

strain and corresponds to a higher value of the stress than at the tetragonal (Bain) path. Based on these considerations, we would expect that the ratio of theoretical tensile strengths of the two paths would be, approximately, $5/2.37 = 2.11$. The ratio of our first-principles values ($\sigma_{\mathrm{th}}^{[111]}/\sigma_{\mathrm{th}}^{[001]} = 27.3/12.7 = 2.15$) agrees well with this estimate corroborating our explanation based on symmetry-dictated extrema. Thus, in a similar way to the explanation given by Šob *et al.* (1997a), a marked anisotropy of calculated ideal tensile stresses in the [001] and [111] loading directions may be understood in terms of structural energy differences of nearby higher-symmetry structures occurring along the deformation path.

From table 1 we may see that there is also a correlation between Young's moduli along the [001] and [111] directions and the ideal tensile strengths for these directions. Namely, $Y^{[111]}$ is about twice $Y^{[001]}$, similarly to the fact that $\sigma_{\mathrm{th}}^{[111]}$ is about twice $\sigma_{\mathrm{th}}^{[001]}$. This relation may be understood on the basis of the following considerations. Young's modulus Y is proportional to the curvature of the E versus ε curve in the ground state. Its higher value indicates that a higher value of the slope of the curve at the inflection point (proportional to the theoretical tensile strength) may be expected. Indeed, the ratio of the Young's moduli $Y^{[111]}/Y^{[001]} = 1.84$ is quite close to the ratio of the theoretical tensile strengths (2.15). A similar relation between the tetragonal shear modulus C' and the structural energy difference $|E_{\mathrm{fcc}} - E_{\mathrm{bcc}}|$ for some cubic transition metals was observed by Wills *et al.* (1992).

The stresses calculated using equation (1) for tensile tests and equation (2) for hydrostatic tension are displayed in figure 1 (*b*). The maximum values corresponding to the inflection points on the total energy dependences (see figure 1 (*a*)) are equal to the theoretical tensile strengths provided that no other instability (soft phonon modes, etc.) appears before reaching the inflection. In the case of iron with its large variety of various magnetic phases, another instability may originate from transitions between various magnetic phases. However, for both [001] and [111] directions of loading we proved that no such transition occurs before the inflection point configuration has been reached (Friák *et al.* 2001c, Šob *et al.* 2003). The values of theoretical tensile strength in [001] and [111] directions are summarized in table 2 in comparison with values determined theoretically for other materials. Non-relaxed calculations are also included; the corresponding values are denoted by a superscript *a*.

The value of the theoretical tensile strength for iron for uniaxial loading in [001] direction, amounting to 12.7 GPa and reported already in our previous work (Friák *et al.* 2001b), is not very different from the value of 14.2 GPa found by Clatterbuck *et al.* (2002). The value of the theoretical strength for loading in [111] direction, namely 27.3 GPa, is nearly equal to that obtained for hydrostatic loading (27.9 GPa). The reason for this parallelism is not clear at present.

The relative changes in atomic volume and the dependences of magnetic moment of ferromagnetic iron per atom on elongation are shown in figures 1 (*c*) and (*d*) respectively. In the neighbourhood of the ground-state structure the atomic volume increases with increasing elongation but exhibits a more complex behaviour at larger deformations. For hydrostatically loaded states, the magnetic moment shows a monotonic increase with increasing volume (in agreement with the work of, for example, Herper *et al.* (1999)) but for tensile test simulations it exhibits local extrema at points of both higher-symmetry structures (maxima for fcc and sc structures) as well as at other points along the studied paths. Let us note that the increase in the magnetic moment with deformation in the neighbourhood of the bcc ground

Table 2. Theoretical tensile strength σ_{th} calculated *ab initio*.

Material	Structure	Direction	σ_{th} (GPa)	Reference
Fe	A2	[111]	27.3	This work
		[001]	12.7	Friák *et al.* (2001b), this work
		[001]	14.2	Clatterbuck *et al.* (2002)
W	A2	[001]	28.9	Šob *et al.* (1997*a*)
		[001]	29.5	Roundy *et al.* (2001)
		[111]	40.1	Šob *et al.* (1997a)
		[110]	54.3	Šob *et al.* (1997a)
Al	A1	[001]	12.1	Li and Wang (1998)
		[111]	11.05	Li and Wang (1998)
		[111]	11[a]	Ogata and Kitagawa (1999)
Cu	A1	[001]	55[a], 32[a]	Esposito *et al.* (1980)
		[001]	33	Šob *et al.* (1998a)
		[110]	31	Šob *et al.* (1998a)
		[111]	29	Šob *et al.* (1998a)
Diamond	A4	[111]	90	Telling *et al.* (2000)
		[111]	95	Roundy and Cohen (2001)
		[001]	225	Telling *et al.* (2000)
		[110]	130	Telling *et al.* (2000)
Si	A4	[111]	22	Roundy and Cohen (2001)
Ge	A4	[111]	14	Roundy and Cohen (2001)
Nb	A2	[001]	13.1	Luo *et al.* (2002)
Mo	A2	[001]	28.8	Luo *et al.* (2002)
TiC	B1	[001]	44	Price *et al.* (1992)
NiAl	B2	[001]	46	Šob *et al.* (1998a,b)
NiAl	B2	[111]	25	Šob *et al.* (1998a,b)
β-SiC	B3 (3C)	[001]	101	Li and Wang (1999)
β-SiC	B3 (3C)	[111]	50.8	Li and Wang (1999)
AlN	B4	[0001]	50[a]	Ogata and Kitagawa (1999)
$MoSi_2$	$C11_b$	[001]	37	Friák *et al.* (2001a)
WSi_2	$C11_b$	[001]	38	Friák *et al.* (2001a)
β-Si_3N_4	$P6_3/m$	[100]	72.2[a]	Ogata *et al.* (2001)
		[100]	57	Ogata *et al.* (2003)
		[001]	75.0[a]	Ogata *et al.* (2001)
		[001]	55	Ogata *et al.* (2003)
Crystalline Si_3N_4	$Fd\bar{3}m$	[001]	45	Kocer *et al.* (2003)

[a]The perpendicular dimensions of the sample were not relaxed during the calculations (no Poisson contraction allowed).

state in the case of uniaxial tensile tests is also connected with increasing volume (cf. figure 1 (*c*) and (*d*)).

§4. Conclusions

In recent years, *ab initio* electronic structure calculations have progressed from determination of equilibrium characteristics of materials, such as lattice parameters, single-crystal elastic moduli and equations of state, to studies of attributes and parameters corresponding to states and configurations far away from equilibrium. One such quantity is the theoretical (ideal) strength of materials. Since it represents the upper limit of stresses that the material may sustain, its knowledge has important implications for understanding the behaviour of solids at the limits of structural stability. Furthermore, it constitutes an important parameter for the construction

of reliable semiempirical interatomic potentials needed for large-scale atomistic modelling of structures that may contain highly strained regions.

In this paper, we presented simulations of the tensile test in ideal crystals of ferromagnetic bcc iron loaded along [001] and [111] axes, using the first-principles full-potential electronic structure calculations within the generalized gradient approximation. The theoretical tensile strengths of iron found in this study are 12.7 GPa for [001] and 27.3 GPa for [111] directions of loading. This marked directional anisotropy of the theoretical tensile strength is apparently related to the presence of distinct symmetry-dictated extrema of the energy along the different deformation paths. The isotropic hydrostatic tension was also analysed and theoretical tensile strength of iron for this case was found to be 27.9 GPa, very close to the value for uniaxial [111] loading. These calculations also reveal that iron keeps its ferromagnetic order up to the strains corresponding to the ideal strength limit. Moreover, with increasing tensile deformation, the magnetic moment increases. This is presumably commensurate with the magnetovolume effects, since the volume per atom also increases. In fact, the increase in the magnetic moment is fastest for the hydrostatic tension when it is accompanied by the fastest increase in the atomic volume.

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