Estimation of the ideal fracture strength between two identical semi-infinite jellia

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We describe an interpolation procedure which allows an estimation of the maximum cohesive force (ideal fracture strength) F_m between two identical semi-infinite jellia. To this purpose use is made of the limiting form of the force $F(z)$ at small and at large distance z, and of the surface energy ε_s of a single semi-infinite jellium. We rely on model calculations of the force in the two limits, and take the surface energy from the available literature.

The study of the interaction force between two solids is of basic importance to understand the physics of the cohesion or adhesion at interfaces and of the cleavage of solids. The jellium model often serves as a first step in the investigation on metallic interfaces. Thus, the adhesive force between two touching semi-infinite jellia (bijellic interface)[1-4] and the corresponding linear force constant[1,2] have been recently reconsidered.[5-15]

In this paper, we focus on the cleavage force $F(z)$ between two identical semi-infinite jellia at distance z. We propose to interpolate $F(z)$ between the known small and large distance functional forms, adapting to the present case an idea originally due to Kohn and Yaniv.[16] To this purpose (i) we recalculate the linear force constant A, (ii) we evaluate the quadratic force constant B and the van der Waals coefficient C, and (iii) we make use of the surface energy ε_s of a semi-infinite jellium.[17-19] In such a manner we are able to obtain an estimate of the maximum cohesive force F_m, which should be more reliable than that obtained with earlier simpler interpolation formulas.[16,7] We remark that the so-called ideal fracture strength F_m constitutes—for real crystals—an important input parameter for theories dealing with bond stretching and crack propagation.

The interface between two semi-infinite jellia at distance z and with equal density n can be characterized by an interfacial energy (per unit area) $\varepsilon_i(z)$ and a cohesive force (per unit area) of magnitude $F(z)$. The interfacial energy (see Fig. 1) can be defined as the work needed to separate at distance z two semi-infinite jellia initially in contact. This requires the application of a cleavage force which just compensates the cohesive force. Thus,

$$F(z) = \frac{d\varepsilon_i(z)}{dz} \ , \quad \varepsilon_i(0) = 0, \quad \varepsilon_i(\infty) = 2\varepsilon_s \ , \tag{1}$$

where ε_s is the surface energy of a semi-infinite jellium.

The functional form of the cohesive force $F(z)$ is not completely known. However,

$$F(z) = \begin{cases} F_0 + Az + Bz^2 + \cdots & \text{as } z \to 0 \qquad (2) \\ C/z^3 + O(1/z^4) & \text{as } z \to \infty \ . \qquad (3) \end{cases}$$

One also knows that the zero-separation force F is related to the bulk pressure of the homogeneous electron gas[1,2] with density n [$\equiv (4\pi r_s^3 a_0^3/3)^{-1}$] and bulk energy (per particle) $\varepsilon(n)$,

$$F_0 = -n^2 \frac{d\varepsilon(n)}{dn} > 0; \tag{4}$$

therefore, it vanishes at $r_s = r_s^* \simeq 3.4$, as is clear from Fig. 2. Here, r_s is the Wigner-Seitz sphere radius in units of Bohr radii a_0. From Eqs. (2)–(4) and the fact that $C > 0$ (see below), it follows that for $r_s < r_s^*$ the cohesive force $F(z)$ vanishes at some z_0, with a linear force constant $F'(z_0)$, and has its maximum F_m (ideal or theoretical fracture strength) at a separation z_m (see Fig. 3).

The linear force constant A can be expressed in terms of the static dielectric function $\epsilon(q)$ of the homogeneous

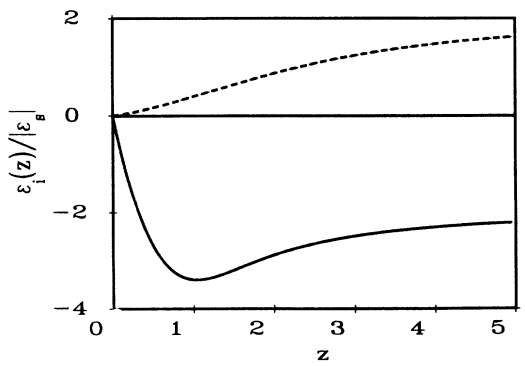

FIG. 1. Interface energy $\varepsilon_i(z)$ vs separation z for two values of r_s. Solid line, $r_s = 2$; dashed line, $r_s = 5$.

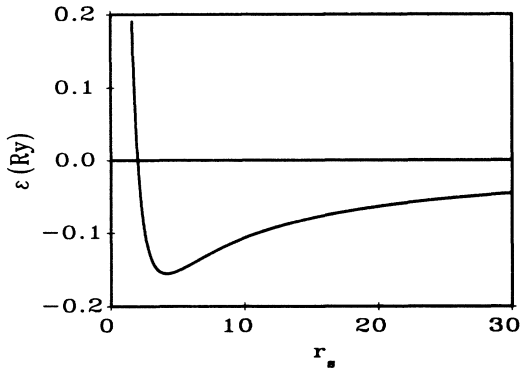

FIG. 2. Energy (per particle) of the homogeneous jellium vs the density parameter r_s (from the parametrization of Ref. 24).

electron gas via[1,2]

$$A = 2n^2e^2 \int_{-\infty}^{\infty} dq \frac{1}{q^2\epsilon(q)} . \tag{5}$$

A convenient representation of $\epsilon(q)$ is[20,21]

$$\epsilon(q) = 1 - \frac{v(q)\chi_0(q)}{1 + v(q)G(q)\chi_0(q)} , \tag{6}$$

with $v(q) = 4\pi e^2/q^2$, $\chi_0(q)$ the Lindhard function and $G(q)$ the local-field function, measuring exchange and correlation effects beyond the Bohm-Pines random-phase-approximation (RPA) [$G(q) = 0$]. The quadratic force constant B, on the other hand, can be obtained from a study of the bijellic interface for small separations.[22] Finally, the van der Waals coefficient C is given by[23]

$$C = \frac{\hbar}{16\pi^2} \int_0^{\infty} du \int_0^{\infty} ds\, s^2 \left[\left(\frac{\epsilon(0,iu)+1}{\epsilon(0,iu)-1} \right)^2 e^s - 1 \right]^{-1} , \tag{7}$$

with $\epsilon(q,\omega)$ the dynamical dielectric function.

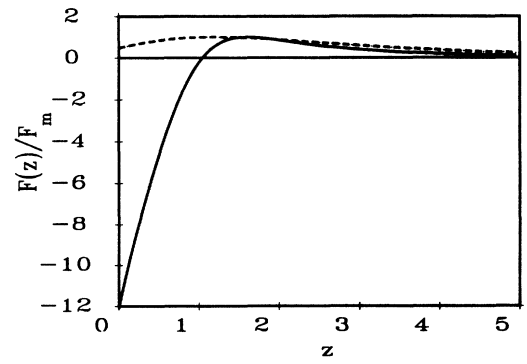

FIG. 3. Cohesive force vs interface separation for two r_s values. Solid line, $r_s = 2$; dashed line, $r_s = 5$. Notice that $F_0 \equiv F(0) = 0$ for $r_s = r_s^*$ (see text).

The various parameters mentioned above are more or less readily available. The zero-separation force F is evaluated from a suitable parametrization[24] of the quantum Monte Carlo data of Ceperley and Alder.[25] A is calculated from Eqs. (5) and (6) using the local field function $G(q)$ of Vashishta and Singwi,[21] which has the correct small q behavior. In fact, it is the small q region that gives the dominant contribution to the integral of Eq. (5). We have also obtained A in an independent manner, resorting to the gradient expansion method (GEM).[2,10,14,22] Expanding the Euler and Poisson equations in powers of z one obtains the analytical expression

$$A = \frac{2\pi e^2 n^2}{q} \frac{\sin(3\delta)}{\sin(2\delta)} , \tag{8}$$

$$q = \left(\frac{2\pi e^2}{\beta(n)} \right)^{1/4} , \quad \delta = \frac{d^2\alpha(n)/dn^2}{4[2\pi e^2\beta(n)]^{1/2}} ,$$

with $\alpha(n) = n\varepsilon(n)$ and $\beta(n) = e^2a_0/72n + \beta_{xc}(n)$, the gradient coefficient. We have taken the exchange and correlation coefficient $\beta_{xc}(n)$ from Ref. 26. The numerical solution of the Euler and Poisson equations for small separation z yields[22]—through numerical differentiation of $F(z)$—a value of A in agreement with that of Eq. (8) and an estimate of the coefficient B. The van der Waals coefficient C is calculated from Eq. (7) with $\epsilon(0,\omega) = 1 - \omega_p^2/\omega^2$, ω_p [$= (4\pi e^2 n/m)^{1/2}$] being the plasma frequency. This yields[16,27]

$$C(r_s) = 1.24 \times 10^{-2} \frac{e^2}{r_s^{3/2} a_0} . \tag{9}$$

Finally, the surface energy ε_s has been taken from the solution of the Kohn-Sham equation for a semi-infinite jellium, obtained with various approximations of the exchange and correlation potential.[17–19]

We interpolate $F(z)$ between the two limiting regimes discussed above by means of a Padé ansatz[28]

$$F(z) = \frac{F_0 + az}{1 + bz + cz^2 + dz^4} . \tag{10}$$

Equations (2) and (3) immediately determine three of the fit parameters according to

$$b = \frac{a - A}{F_0} , \quad c = \frac{A(A-a)}{F_0^2} - \frac{B}{F_0} , \quad d = \frac{a}{C} . \tag{11}$$

The remaining parameter a is readily obtained from the extra condition

TABLE I. Input parameters for the interpolation 10: F_0 in units of $10^{-5}e^2/a_0^4$ from Ref. 4, B in units of $10^{-5}e^2/a_0^6$ from Ref. 22, and C in units of $10^{-3}e^2/a_0$ from Ref. 10.

r_s	F_0	B	C
2	−301	−237	4.38
5	1.21	−0.992	1.11

TABLE II. Ideal fracture strength F_m in units of $10^{-5}e^2/a_0^4$, at two values of r_s and for various choices of the parameters A and ε_s, using the interpolation scheme described in the text. The last two rows give F_m from other calculations (Refs. 1 and 22). A is in units of $10^{-5}e^2/a_0^5$ and ε_s in units of $10^{-5}e^3/a_0^3$. For comparison, the Thomas-Fermi approximation for $\epsilon(q)$ yields (Refs. 6 and 7) A=506,3.28 and the RPA [i.e., $G(q)=0$] yields A=539,3.73 at r_s=2,5, respectively.

	F_m					
	$r_s=2$				$r_s=5$	
ε_s	−64.7[a]	−37.6[b]	−17.8[c]	ε_s	6.42[a]	5.14[c]
A				A		
462[d]	6.47	24.1	46.1	2.38[d]	3.14	2.55
443[e]	7.59	26.5	49.5	2.13[e]	3.05	2.46
		11[f]			2.1[f]	
		22[g]			2.6[g]	

[a] From Ref. 17.
[b] From Ref. 18.
[c] From Ref. 19.
[d] A using the $G(q)$ from Ref. 18.
[e] A from GEM calculations (Ref. 20).
[f] From Ref. 2.
[g] From Ref. 22.

$$\int_0^\infty dz\, F(z) = \varepsilon_i(\infty) - \varepsilon_i(0) = 2\varepsilon_s, \tag{12}$$

which follows from Eq. (1). Clearly, only those solutions of the equation above are accepted for which the denominator in Eq. (10) does not vanish (for $z > 0$). Once all the parameters are known—for a given r_s—the critical values F_m and z_m, and z_0 and $F'(z_0)$ if wanted, can be readily calculated.

The results of the interpolation are considered in detail below for $r_s = 2$ and $r_s = 5$. The parameters F, B, and C are given in Table I. For A and ε_s we have used various estimates, as already mentioned above. Whereas the estimates of A from $\epsilon(q)$ and from the GEM are in fair agreement, there is still a sizable uncertainty on ε_s for small r_s, as obtained from the available Kohn-Sham calculations. In Table II we report the ideal fracture strength F_m obtained from various choices of A and ε_s. Our results for F_m are sensitive to the value of ε_s. Therefore, the reliability of our calculated F_m [as well as that of z_m, $F(z_0)$, z_0] depends on that of the surface energy calculations.

Future work should try to assess the value of ε_s on a firmer ground, through calculations on the semi-infinite jellium. On the other hand, investigations on the force constants A and B will require the study of the slightly cleaved jellium. It should also be possible to calculate B from the knowledge of the linear and of the quadratic response functions for the homogeneous infinite jellium. In this respect it would be interesting to try a RPA for the quadratic response.[29]

In trying a direct comparison of our results with empirically (phenomenologically) estimated data one should remember (i) that jellium can be considered a reasonable model only for low-density simple metals—as far as the surface energy is concerned; (ii) that for real solids the cleavage force starts with $F_0 = 0$, and therefore for a metal with $r_s > r_s^*$ the empirical fracture strength should be compared with $F_m - F_0$, rather than with F; similarly for a metal with $r_s < r_s^*$ the fracture strength separation might be compared with $z_m - z_0$, rather than with z_0.

We notice that the present interpolation scheme can be applied also to interfaces between real solids, if one is able to estimate the values of A, B, C, and of the adhesive energy $\int_0^\infty dz\, F(z)$.

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[1] H. F. Budd and J. Vannimenus, Phys. Rev. Lett. **31**, 1218 (1973).
[2] J. Vannimenus and H. F. Budd, Solid State Commun. **17**, 1291 (1975).
[3] H. F. Budd and J. Vannimenus, Phys. Rev. B **14**, 854 (1976).
[4] J. Heinrichs and N. Kumar, Solid State Commun. **18**, 961 (1976).
[5] N. H. March and B. V. Paranjape, Phys. Rev. B **30**, 3131 (1984).
[6] J. Heinrichs, Phys. Rev. B **32**, 4232 (1985).
[7] P. Streitenberger, Phys. Status Solidi B **135**, 321 (1986).
[8] D. Lehmann and P. Ziesche, Phys. Status Solidi B **135**, 651 (1986).
[9] M. P. Das, R. Kaschner, N. Nafari, and P. Ziesche, Solid State Commun. **63**, 367 (1987).
[10] A. Erlebach, R. Kaschner, and P. Ziesche, Solid State Commun. **65**, 297 (1980).
[11] N. Nafari and M. P. Das, J. Phys. Chem. Solids **49**, 997 (1988).
[12] P. Streitenberger, P. Ziesche, and N. Nafari, Phys. Status Solidi B **152**, 111 (1989); in *Proceedings of the 19th Inter-*

national Symposium on Electronic Structure, edited by P. Ziesche (Technische Universität, Dresden, 1989), p. 238.
[13]R. Kaschner, J. Gräfenstein, and P. Ziesche, No. IC/88/394, International Centre for Theoretical Physics (Trieste) (1988).
[14]P. Ziesche, R. Kaschner, and N. Nafari, Phys. Rev. B **41**, 10 553 (1990).
[15]R. Kaschner, thesis, Technische Universität, Dresden (1989).
[16]W. Kohn and A. Yaniv, Phys. Rev. B **20**, 4948 (1979).
[17]N. D. Lang and W. Kohn, Phys. Rev. B **1**, 4555 (1970).
[18]E. Alvarellos, P. Tarazona, and E. Chacón, Phys. Rev B **33**, 6579 (1986).
[19]E. Chacón and P. Tarazona, Phys. Rev. B **37**, 4020 (1988).
[20]K. S. Singwi, M. P. Tosi, R. H. Land, and A. Sjölander, Phys. Rev. **176**, 589 (1968).
[21]P. Vashishta and K. S. Singwi, Phys. Rev B **6**, 875 (1972).
[22]R. Kaschner and T. Vojta, Z. Phys. (to be published).
[23]E. M. Lifshitz, Zh. Eksp. Teor. Fiz. **29**, 94 (1955) [Sov. Phys.—JETP **2**, 73 (1956)].
[24]S. H. Vosko, L. Wilk, and M. Nusair, Can. J. Phys. **58**, 1200 (1980).
[25]D. M. Ceperley and B. J. Alder, Phys. Rev. Lett. **45**, 567 (1980).
[26]K. H. Lau and W. Kohn, J. Phys. Chem. Solids **37**, 99 (1976).
[27]E. Zaremba, Solid State Commun. **23**, 347 (1977).
[28]If one tries to generalize the otherwise successful interpolation ansatz of Kohn and Yaniv (Refs. 16, 7, and 12) in such a way that it allows both $F_0 > 0$ and $F_0 < 0$ [where $F_0 \equiv F(0)$], i.e., $F(z) = A_0(z - z_0)/[1 + (A_0/C)^{1/2}(z - z_0)^2]^2$, then the corresponding surface energy is always positive in contradiction to the situation for small r_s (Ref. 17).
[29]P. Streitenberger, P. Ziesche, and R. Kaschner (unpublished).