100μm ×126

FIG. 3. SEM photograph of the cavity structures used for leak testing (cross-sectional view).

The quality of our bonds was tested by a cleaving or fracturing technique. To ensure the quality of the bond formed by the abovementioned techniques, wafers of different crystal orientation, and also wafers that were intentionally misaligned, were cleaved and fractured. We have observed that poorly bonded wafers broke irregularly and separated from each other upon fracture, whereas a clean fracture was obtained when a good bond was formed. To check for structural integrity, the bonded wafers were heated to about 1000 °C, and then put on a ceramic block. Attempts to separate the wafers with the sharp edge of a tweezer were unsuccessful.

In order to leak test the Si-to-Si bonds, a wafer containing a micromachined cavity (Fig. 3) was bonded to another wafer after trapping helium in the volume of the cavity with the applied pressure. Leak detection to a sensitivity of 10^{-8} cc/s showed no noticeable leak in the bonded wafers with cavity volume of 3.3×10^{-5} cm^3. We also tested for leaks by pressurizing the bonded wafers to 1.7×10^6 Pa (250 psi) to force He into the cavity, which could then be detected with the leak detector; no leak was observed. These tests indicate to us that this bonding technique could be useful for making hermetically sealed cavities or packages.

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An approximate solution to the scattering integral for general interatomic potentials

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An approximation of the scattering integral is derived by expanding the potential about the distance of closest approach and truncating the expansion so that the integral can be performed analytically. The results are improved by using the approximate integrand only in the region near the closest approach, and assuming zero potential for large distances. The analytical solution, which requires little computation time relative to other solution methods, is shown to yield sufficient accuracy for a wide range of particle energies and impact parameters, using both the Moliere and "Universal" potentials.

The Monte Carlo method is now widely used to predict the transport of energetic ions in solids.[1,2] This numerical simulation method requires repeated calculations of the scattering angle of an ion in collision with the lattice. If these evaluations are simplified, computer time is saved and more particle histories can be simulated. Numerical evaluation of the scattering integral can be time consuming and inaccurate because the integrand is weakly singular at the distance of closest approach, and thus accurate, analytical representations of the scattering angle in a general potential field are

desirable. In this communication, an approximate method for obtaining a closed-form solution of the scattering integral is presented and its region of validity is discussed.

In a two-body collision influenced by a central potential field $V(r)$, the scattering angle is given by[3]

$$\Theta = \pi - \int_\rho^\infty \frac{2p\,dr}{r^2[1 - V(r)/E_0 - p^2/r^2]^{0.5}}, \tag{1}$$

where Θ is the scattering angle, p is the impact parameter, ρ is the distance of closest approach, and E_0 is the particle energy, which is measured in center of mass coordinates, i.e.,

$$E_0 = [M_2/(M_1 + M_2)]E_1, \tag{2}$$

where M_1 and M_2 are the masses of the projectile and target particles, respectively, and E_1 is the projectile energy in lab coordinates. The distance of closest approach, which is the point at which the projectile's radial velocity is zero, is determined from the following equation

$$1 - V(\rho)/E_0 - p^2/\rho^2 = 0. \tag{3}$$

To nondimensionalize the integral, the following substitutions are made

$$x = r/a, \quad \eta = \rho/a, \quad \beta = p/a,$$
$$\epsilon = \frac{aE_0}{Z_1 Z_2 e^2}, \quad V(x) = \frac{Z_1 Z_2 e^2}{ax}\phi(x), \tag{4}$$

where $\phi(x)$ is the screening function and a is the screening length, which depends on the Bohr radius and the atomic numbers of the two particles. Two forms commonly used for the screening length are given by Lindhard, Scharff, and Schiott[4]

$$a = 0.8853\,a_0\,(Z_1^{2/3} + Z_2^{2/3})^{-1/2} \tag{5}$$

and Firsov[5]

$$a = 0.8853\,a_0\,(Z_1^{1/2} + Z_2^{1/2})^{-2/3}, \tag{6}$$

where a_0 is the Bohr radius ($a_0 = 0.529$ Å). The resulting integral is

$$\Theta = \pi - \int_\eta^\infty \frac{2\beta\,dx}{x^2[1 - \phi(x)/\epsilon x - \beta^2/x^2]^{0.5}}, \tag{7}$$

and the nondimensional distance of closest approach η is found from

$$1 - \phi(\eta)/\epsilon\eta - \beta^2/\eta^2 = 0. \tag{8}$$

As seen from Eq. (8), the integrand in Eq. (7) is singular at $x = \eta$, so the choice of numerical integration scheme is limited and requires many quadrature points. Hence, an analytical approach is desirable. In the discussions that follow, both the Moliere and Universal screening functions will be used to demonstrate the usefulness of closed-form approximations. The Moliere screening function[6] is defined by

$$\phi(x) = 0.35\,e^{-0.3x} + 0.55\,e^{-1.2x} + 0.1\,e^{-6x}, \tag{9}$$

and the Universal screening function, which was recently developed by Ziegler, Biersack, and Littmark,[7] is given by

$$\phi(x) = 0.1818\,e^{-3.2x} + 0.5099\,e^{-0.9423x}$$
$$+ 0.2802\,e^{-0.4028x} + 0.02817\,e^{-0.2016x}, \tag{10}$$

where the screening radius is modified to

$$a = 0.8854\,a_0(Z_1^{0.23} + Z_2^{0.23})^{-1/2}. \tag{11}$$

In general, closed-form solutions for the integration of Eq. (7) are not available, so approximations are necessary to obtain analytical formulas for the scattering angle. The solution approach used here expands the screening function about the distance of closest approach (where the integrand is singular) and truncates the series to obtain a closed-form solution. To facilitate this approach, an additional substitution is introduced

$$w = 1/\eta - 1/x, \tag{12}$$

which leads to

$$\Theta = \pi - 2\beta I,$$
$$I = \int_0^{1/\eta} h(w)\,dw, \tag{13}$$

and

$$h(w)$$
$$= \left(1 - \frac{\eta^2}{\beta^2} - \frac{\phi(x)}{\epsilon\eta} + \frac{\phi(x)w}{\epsilon} + \frac{2\beta^2 w}{\eta} - \beta^2 w^2\right)^{-0.5}, \tag{14}$$

or, using Eq. (8),

$$h(w) = \left(\frac{\phi(\eta) - \phi(x)}{\epsilon\eta} + \frac{\phi(x)w}{\epsilon} + \frac{2\beta^2 w}{\eta} - \beta^2 w^2\right)^{-0.5}. \tag{15}$$

The screening function is expanded about $w = 0$ to yield

$$\phi(x) = \phi(\eta) + w\eta^2 \frac{d\phi(x)}{dx}\Big|_{x=\eta}$$
$$+ w^2\eta^3\left(\frac{d\phi(x)}{dx}\Big|_{x=\eta} + \frac{\eta}{2}\frac{d^2\phi(x)}{dx^2}\Big|_{x=\eta}\right)$$
$$+ O(w^3) \quad w \to 0, \tag{16}$$

and the integrand becomes

$$h(w) \simeq g(w),$$

where $\tag{17}$

$$g(w) = (Kw - Qw^2)^{-0.5}.$$

The constants K and Q are given by

$$K = \eta + \frac{\beta^2}{\eta} - \frac{\eta}{\epsilon}\frac{d\phi(x)}{dx}\Big|_{x=\eta}$$

and $\tag{18}$

$$Q = \beta^2 + \frac{\eta^3}{2\epsilon}\frac{d^2\phi(x)}{dx^2}\Big|_{x=\eta}.$$

Because the screening function was expanded about the distance of closest approach, the approximation of Eq. (17) will be least accurate at $x = \infty$. In order to improve the closed-form approximation to the scattering angle, another representation for $\phi(x)$ is needed for large x (w near $1/\eta$). An expansion is inadvisable, because most interatomic potentials are not analytic at $x = \infty$, and thus the screening function will be assumed to be zero for all x greater than an assigned value, and the scattering integral will be divided into two intervals. Hence,

Blanchard, Ghoniem, and Chou

$$I = \int_0^c h(w)\, dw + \int_c^{1/\eta} h(w)\, dw,$$

or

$$I \simeq \int_0^c g(w)\, dw + \int_c^{1/\eta} f(w)\, dw, \tag{19}$$

where $g(w)$ is given by Eq. (17) and

$$f(w) = \left(1 - \frac{\beta^2}{\eta^2} + \frac{2\beta^2 w}{\eta} - \beta^2 w^2\right)^{-0.5}. \tag{20}$$

The choice for c, the point at which the integral is divided, is somewhat arbitrary. By varying this point and comparing the results to the numerical calculations of the scattering angle, the optimal split was found to depend only on the impact parameter and the distance of closest approach:

$$c = \alpha/\eta,$$

where $\tag{21}$

$$\alpha = 0.42 - \beta/80.$$

The scattering angle is now given by

$$\Theta \simeq 2\cos^{-1}\left(\frac{\beta}{\eta}(1-\alpha)\right) - \frac{2\beta}{\sqrt{Q}}\cos^{-1}\left(1 - \frac{2\alpha Q}{K\eta}\right). \tag{22}$$

The results for this approximation are shown in Table I, where the numerical integrations were performed using the quadrature method of the IMSL library.[8] The accuracy is reasonable, with errors of less than 10% for $\epsilon = 0.0002$ and a maximum error of about 23% ($\beta = 17$, $\epsilon = 2$, Universal screening function). Considering the wide range of impact parameters and energies shown in the table, Eq. (22) gives a useful representation of the scattering angle for many applications. The approximate result (using the Universal screening function) is valid only for $\epsilon > 7.3 \times 10^{-6}$ in a near head-on collision ($\beta \simeq 0$) and for $\epsilon > 1.3 \times 10^{-9}$ for glancing collisions ($\beta > 20$), because for very small reduced energy the argument of the second inverse cosine in Eq. (22) becomes less than -1.

TABLE I. Scattering angle (in radians).

| β	ϵ	Moliere		Universal	
		numerical	analytical	numerical	analytical
1	0.000 02	3.04	not valid	3.03	3.07
7	0.000 02	2.41	2.67	2.35	2.49
17	0.000 02	1.34	1.41	1.26	1.26
1	0.0002	2.99	3.03	2.96	3.00
7	0.0002	2.07	2.21	1.90	1.96
17	0.0002	0.690	0.689	0.517	0.524
1	0.002	2.87	2.87	2.82	2.82
7	0.002	1.40	1.40	1.13	1.13
17	0.002	0.157	0.158	0.0896	0.0916
1	0.02	2.52	2.52	2.45	2.46
7	0.02	0.457	0.465	0.301	0.305
17	0.02	0.0186	0.0188	0.009 82	0.010 00
1	0.2	1.44	1.47	1.43	1.45
7	0.2	0.0621	0.0637	0.0377	0.0383
17	0.2	0.001 93	0.001 91	0.001 02	0.001 00
1	2.0	0.277	0.295	0.277	0.293
7	2.0	0.006 46	0.006 62	0.003 88	0.003 94
17	2.0	0.000 219	0.000 192	0.000 131	0.000 101
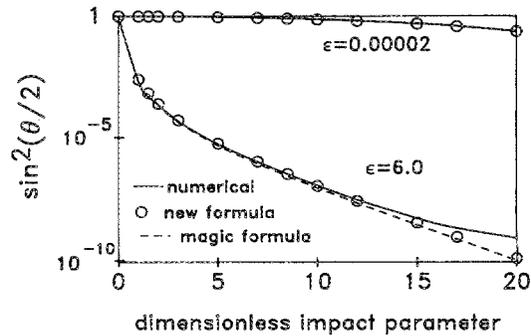
FIG. 1. Comparison of three methods for calculating the scattering angle.

The usefulness of Eq. (22) is shown in Figs. 1 and 2, which compare the results of the analytical approximation to numerical results and to the so-called Magic Formula.[9] The Magic Formula, another approximation to the scattering angle, avoids the need for repeated numerical integrations by fitting a few numerical calculations to an assumed function. Calculations on a Cray-1 computer show that the computational requirements of this formula are comparable to those of the approximation developed in this communication. The new approximation, however, is more versatile because it disregards the empirical approach in favor of a more physical derivation based on the behavior of the potential. This allows calculations for virtually any potential.

Figure 1 shows that on a log scale, the two approximations are indiscernible from the numerical calculations over the whole range shown. In Fig. 2, results for the Moliere and Universal potentials are compared for a reduced energy of 0.000 02, using numerical integration and Eq. (22). It is evident that errors in the approximation are small compared to differences in the representations of the potential. Hence, this new approximation, with its decreased computational demands, should be useful as a representation of the scattering angle.

The scattering integral can be approximated by expanding the potential about the distance of closest approach before integrating the resulting integrand over a portion of the interval, and assuming that there is zero potential over the rest of the interval. This is successful because the integral is
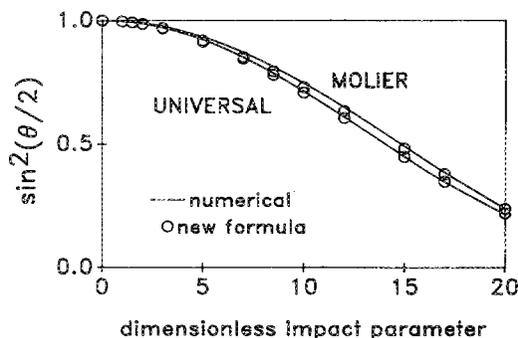

FIG. 2. Comparison of scattering angles calculated using two different potentials for $\epsilon = 0.000\ 02$.

dominated by the influence of the potential in the neighborhood of the distance of closest approach, unless the particle energy is extremely small. This closed-form approach yields accurate results at a significant savings in computation time as compared to numerical quadrature methods, and it is useful over a wide range of energies and impact parameters.

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Nonequilibrium ionization of nitrogen: The role of stepwise ionization from metastable states in the presence of superelastic electronic collisions

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Electron impact ionization rate coefficients involving N_2 metastable electronic states have been calculated in discharge and postdischarge conditions by using the electron energy distribution functions which take into account both the presence of superelastic electronic (SEC) and vibrational (SVC) collisions [J. Appl. Phys. **59**, 4004 (1986)]. The results show that stepwise ionization from metastable states can overcome the corresponding rates from the ground state especially in the absence of SVC. Finally, a comparison of the present results with those coming from associative ionization involving metastable electronic and vibrational states is presented and discussed.

Nitrogen ionization under nonequilibrium conditions has been extensively studied[1-4] in these last years due to the importance of this process in different fields of plasma technology. Different mechanisms have been proposed to explain the process. In particular we want to mention

(a) Electron impact ionization collisions[1,2]:

$$e + N_2(X,v) \rightarrow e + N_2^+ + e, \qquad (1)$$

from the ground electronic states of N_2, i.e., $N_2(X,v) \equiv N_2(X\,{}^1\Sigma_g^+)$ including the different vibrational levels of X state (i.e., levels v).

(b) Electron impact ionization collisions from electronically excited states, in particular from metastable states:

$$e + N_2(A) \rightarrow e + N_2^+ + e, \qquad (2)$$

$$e + N_2(a') \rightarrow e + N_2^+ + e, \qquad (3)$$
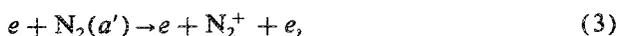
where A and a' represent, respectively, the $A\,{}^3\Sigma_u^+$ and $a'\,{}^1\Sigma_u^-$ metastable states.

(c) Heavy particle ionization collisions involving metastable states[1,3]:

$$N_2(A) + N_2(a') \rightarrow N_2^+ + N_2 + e, \qquad (4)$$

$$N_2(a') + N_2(a') \rightarrow N_2^+ + N_2 + e. \qquad (5)$$
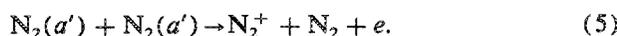
(d) Heavy particle ionization collisions involving vibrationally excited nitrogen levels of the ground electronic state[1,4]:

$$N_2(X,v) + N_2(X,w) \rightarrow N_4^+ + e$$
$$\qquad \qquad \rightarrow N_2^+ + N_2 + e. \qquad (6)$$
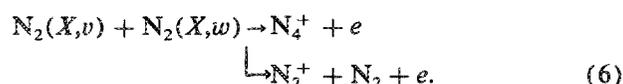
(e) Heavy particle ionization collisions involving metastable and vibrationally excited states[1,4]:

$$N_2(X,v) + N_2(a'') \rightarrow N_2^+ + N_2 + e \quad v \geqslant 12, \qquad (7)$$

$$N_2(X,v) + N_2(a') \rightarrow N_2^+ + N_2 + e \quad v \geqslant 25, \qquad (8)$$
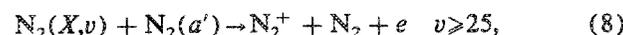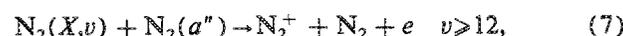
where $N_2(a'') \equiv N_2(a''\,{}^1\Sigma_g^+)$.

The dominance of a given mechanism depends on the particular conditions studied as well as on the adopted rate coefficients, which in general are poorly known.

At low values of the reduced electric field $E/N(E/N \leqslant 5 \times 10^{-16} \text{ V cm}^2)$ reaction (1) gives too small ionization rates as compared with the experimental values,[1] so that one is forced to utilize other mechanisms to explain the experimental rates.

Two tendencies are essentially present in the literature, one which prefers to explain the experimental data (espe-