$$\times \sum_G \left| \frac{\vec{G}\cdot\vec{E}(\pm\vec{G}\pm\vec{q}_o)}{4\pi e} \right|^2 \Delta_{\vec{q}\pm\vec{q}_o\pm\vec{G}} \,. \quad (6)$$

Inelastic surface scattering. Because of the discontinuity in the unperturbed electronic density and the optical dielectric function, the divergence of the primary electric field is nonzero at the surface of a crystal if the incident wave has a component polarized perpendicular to the surface. If E_z is the normal component of the optical field inside the surface at $z=0$, we have[5]

$$n_s(\vec{r},t) \simeq \frac{1-\epsilon(\omega_o)}{4\pi e} \left[E_z \delta(z) e^{i(\vec{q}_{ot}\cdot\vec{r}-\omega_o t)} + \text{c.c.}\right], \quad (7)$$

where $\vec{q}_{ot}$ is the tangential component of the optical wave vector. Thus we have

$$\frac{d\sigma}{d\Omega} = r_0^2 \left|\hat{e}_s\cdot\hat{e}_i\right|^2 \frac{\omega_s}{\omega_i} \left[1-\epsilon(\omega)\right]^2 \times \left|\frac{E_z}{4\pi e}\right|^2 A^2 \delta_{\vec{q}_t\pm\vec{q}_{ot},0} \,, \quad (8)$$

where A is the area of the surface.

Note that the surface term, unlike the Bragg terms, is peaked only for tangential directions of $\vec{q}_s$. In comparing the integrated intensities, we will consider a solid angle which just encompasses a Bragg beam. We find

$$\frac{d\sigma(\text{Bragg inel})}{d\sigma(\text{el})} \simeq \left|(4\pi e n_o)^{-1}\vec{G}\cdot\vec{E}(\vec{q}_o+\vec{G},\omega_o)\right|^2$$

and

$$\frac{d\sigma(\text{surf})}{d\sigma(\text{Bragg inel})} \simeq \frac{q_s\left|E_z(\vec{q}_o,\omega_o)\right|^2}{L_z\left|\vec{G}\cdot\vec{E}(\vec{q}_o+\vec{G},\omega_o)\right|^2} \,.$$

L_z is the thickness of the crystal. We can know $E(\vec{q}_o+\vec{G},\omega_o)/E(\vec{q}_o,\omega_o)$ exactly only if we have the value of the microscopic dielectric tensor. However, this ratio is expected[6] to be of order 10^{-2}–10^{-3}. Thus, the elastic Bragg peak is dominant unless $E(\vec{q}_o,\omega_o) \sim 10^6$–$10^7$ esu. The surface term becomes important in comparison to the inelastic Bragg term for crystals thinner than 10^{-2}–10^{-4} cm. For a solid made of crystallites of this size, the surface term cannot be neglected. Note also that the condition on L_z is relaxed for more realistic (i.e., larger) solid angles used in experiments. In the above estimates, we have assumed that q_s and G are of order $10^8\,\text{cm}^{-1}$ and $n_0 \sim 10^{22}\,\text{cm}^{-3}$.

Finally, we remark that surface ($\nabla\cdot E$ term at the surface) and local field ($\nabla\cdot E$ term in the bulk) corrections are negligible when one is considering the mixing of two x-ray photons.[7]

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Monte Carlo Study of the Elastic Constants of Compressed Ar†

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A Monte Carlo calculation of the elastic constants of solid Ar at 80 °K and near zero pressure has been reported by Klein and Murphy. This calculation employed the Bobetic-Barker Ar_2 pair potential and included a correction both for three-body forces and quantum effects. The present note extends the previously calculated elastic constants to include the volume dependence at 80 °K and the temperature dependence at 21.99 $\text{cm}^3\,\text{mole}^{-1}$. Comparison is made, where possible, with the scant experimental data.

Using lasers it is now possible to measure the elastic constants of rare-gas solids either by spontaneous[1] or stimulated Brillouin scattering[2] (SBS). The feasibility of studying the isothermal pressure dependence of SBS has also been demonstrated.[3] Moreover, with currently available

TABLE I. Monte Carlo values for the elastic constants[a] of solid Ar (in kbar) based upon the BB Ar_2 pair potential and ATM three-body force.[b]

	Two body (BB)	Three body (ATM)	Total	V and T
c_{11}^s	22.81	2.13	24.94	$V = 24.43$ cm^3 mole^{-1}, $T = 80$ °K
$c_{11} - c_{12}$	8.73	−0.09	8.64	
c_{44}	11.77	0	11.77	
B_T	11.02	2.19	13.21	
p	−0.476	0.549	0.073	
c_{11}^s	40.01	2.92	42.93	$V = 22.60$ cm^3 mole^{-1}, $T = 80$ °K
$c_{11} - c_{12}$	14.78	−0.11	14.67	
	20.04	0	20.04	
B_T	24.16	2.99	27.15	
p	0.825	0.750	1.575	
c_{11}^s	48.19	3.25	51.44	$V = 21.99$ cm^3 mole^{-1}, $T = 80$ °K
$c_{11} - c_{12}$	17.57	−0.12	17.45	
c_{44}	24.22	0	24.22	
B_T	30.09	3.33	33.42	
p	1.565	0.836	2.401	
c_{11}^s	52.48	3.25	55.73	$V = 21.99$ cm^3 mole^{-1}, $T = 180$ °K
$c_{11} - c_{12}$	12.53	−0.12	12.41	
c_{44}	21.25	0	21.25	
B_T	31.43	3.33	34.76	
p	4.355	0.836	5.191	

[a]Our elastic constants c_{ij} are the same as the B_{ij} of D. C. Wallace [Phys. Rev. 162, 776 (1967)] and are the usual generalized Birch coefficients appropriate to cubic materials under isotropic stress.

[b]The probable errors in the adiabatic constants is ± 2%, while for B_T it is likely ± 3%. For p the statistical error is about ± 20 bar, but a further systematic error of about +25 bar most likely arises through the quantum correction (see Ref. 7 for details).

technology a measurement of the isochoric temperature dependence is, in principle, also possible.[4] This, together with the improvement of the conventional equation-of-state technique[5] as well as isochoric studies,[6] makes it desirable to have some predictions for the elastic properties of solid Ar for volumes and temperatures away from the vapor-pressure line. This is the purpose of the present note, which therefore complements both the Monte Carlo elastic-constant study of Klein and Murphy[7] and the melting-line investigation of Barker and Klein.[8]

Details of the calculations are identical to that of Klein and Murphy[7] and are thus not reproduced here. The results are collected in Table I. The Ar_2 pair potential used was that of Bobetic and Barker[9] (BB), and three-body force is approximated by the Axilrod–Teller–Muto (ATM) form.[7] It should be recalled that the pair potential is in part parametrized to zero-temperature solid-state properties.[9] Unfortunately, it is not possible to compare the calculated elastic constants directly with experiment. However, from the isochoric calculations of Table I, we find $(dp/dT)_V = 27.9$ bar °K^{-1} for $V = 21.99$ cm^3 mole^{-1}, which agrees well with the work of Benson and Daniels.[6] The pVT melting-line studies of Crawford and Daniels[10] can be compared with the present calculations, if we correct the latter using the calculated bulk modulus of Table I and the value of $(dp/dT)_V$ given above. Thus we find for $V = 22.09$ cm^{3}mole^{-1} and $T = 180.15$ °K a calculated pressure $p = 5029 \pm 20$ bar, whereas Crawford and Daniels found experimentally $p = 4999 \pm 7$ bar. Independently, Baker and Klein obtained by Monte Carlo methods $p = 5036 \pm 10$ bar for the BB potential with three-body forces at the same V and T.

Meixner *et al.*[2] measured the pressure dependence of SBS for longitudinal sound propagating in the (110) plane at 25° to the [111] axis. The zero-pressure sound velocity v_0 was found to be 1424 ± 5 m sec^{-1} and the pressure coefficient $d\ln v/dp = 0.22 \pm 0.01$ kbar^{-1} at 77 °K. The experimental[11] isothermal bulk modulus at 77.7 °K is 12.7 ± 0.6 kbar so that $-(d\ln v/d\ln V) = 2.79 \pm 0.27$ and hence[12] the mode Grüneisen parameter $\gamma = 3.12 \pm 0.27$.

From Table I we estimate $v_0 \sim 1440$ m sec^{-1} at 80 °K and

$$\gamma = \frac{1}{2}\frac{d\ln c_{ij}}{d\ln V} - \frac{1}{6} = 3.22 \pm 0.27,$$

where c_{ij} is the appropriate elastic constant and the error estimate is based upon a possible 2% error in the individual adiabatic constants of Table I. While the agreement with available pressure ex-

periments is encouraging, further experiments would be most helpful in pointing out possible inadequacies in the pair potential[13] or the approximation for the many-body forces.

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Solution to One-Dimensional Schrödinger Equation for an Arbitrary Potential; Application to Radial Equation in Three Dimensions*

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The work of Reading and Sigel on the solution of the one-dimensional Schrödinger equation for a particle moving in the presence of a collection of δ-function potentials of arbitrary strength and position is generalized so that any arbitrary potential $V(x)$ can be handled. A close connection is shown to exist between the methods described in this note and those, involving Jost functions, which have been developed for handling the radial Schrödinger equation in three dimensions.

INTRODUCTION

In a recent paper[1] by Reading and the present author, a method was developed for the determination of the wave functions for an electron moving in a one-dimensional array of δ-function potentials. In this paper the fundamental simplicity of the technique elaborated in Ref. 1 will be demonstrated by at first formally constructing the solution of the one-dimensional Schrödinger equation for the general case of an arbitrary potential $V(x)$. The details of the δ-function potential, as will be pointed out, need be considered only after most of the derivation is carried out. A close connection will be demonstrated to exist between the techniques presented here and those, involving Jost functions, which are used in scattering theory to obtain a (formal) solution to the radial Schrödinger equation.

To start, take the integral form of the Schrödinger equation (as in Ref. 1)

$$\psi(x) = (1/2ki)\int dx'\, e^{ik|x-x'|}V(x')\psi(x') + Ae^{ikx} + Be^{-ikx}, \tag{1}$$

where $k = E^{1/2}$ (E is the energy). Next, define

$$S(\pm) = \int_{-\infty}^{\infty} dx\ \alpha(x)\psi(x)e^{\pm ikx}, \tag{2}$$

where $\alpha(x) = (-2ik)^{-1}V(x)$ and assume here, and in the following, the necessary convergence. By use of (2), Eq. (1) can be rewritten as

$$\psi(x) = [B - S(+)]\,e^{-ikx} + Ae^{+ikx} - \int_{-\infty}^{x} dx'\,(e^{ik(x-x')} - e^{-ik(x-x')})\,\alpha(x')\psi(x'). \tag{3}$$

Just as in Ref. 1, at first, $S(+)$ *can be treated as a parameter.* The solution to (3), which is clearly