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High-accuracy structure-factor measurements in germanium

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Structure factors F_h of five reflections in the range $0.15 \leq \sin\theta/\lambda \leq 1.07$ Å^{-1} were measured in germanium. An accuracy of ≤ 20 millielectron per atom was achieved for all values except one. This represents 1 order of magnitude improvement over previous measurements for the three highest-order F_h. Measurements were done using the W $K\alpha_1$ line ($E = 59.3$ keV) and a monolithic thin-crystal Laue-case diffractometer, the rocking curves of which were computer fitted to yield F_h. Good agreement is obtained with previous measurements, where available. The bonding contribution to F_{111} is found to be larger than predicted by *ab initio* calculations. No evidence is found for an anharmonic contribution to the atomic potential, within the accuracy of the measurements. This is in keeping with x-ray results for silicon, but in contrast with neutron and x-ray "forbidden" reflection measurements. The Debye parameter $B = (0.5661 \pm 0.0026)$ Å^2 derived from our data is in excellent agreement with older results.

I. INTRODUCTION

Due to their simple structure, and availability as large, nearly perfect single crystals, silicon and germanium have been a testing ground of choice for theoretical models of binding,[1-3] band structure,[4-6] thermal motion,[7-9] and the scattering of radiation in crystalline materials. The millielectron-level accuracy measurements of the low-order structure factors of silicon by Kato and coworkers,[10] Teworte and Bonse,[11] and, in particular, Hart and coworkers,[12] allowed for the detection of a ~7% expansion of the valence shell, the determination of the nonspherical distortions of free-atom charge distribution, the harmonic vibration amplitude of the atom, and the upper limit to the anharmonic term in the effective one-atom potential.[13] Furthermore, the high-order structure factor measurements of the present authors[9,14] further reduced the upper limit on the anharmonic term in the potential and supplied evidence for a nonrigid thermal motion of the crystal-bound silicon atom.

By contrast, germanium, although expected to exhibit larger thermal and atomic nonrigidity effects due to its higher atomic number and lower Debye temperature, was much less investigated experimentally. Only three studies having accuracies better than 100 millielectrons were published.[15-17] Furthermore, they are restricted to reflections with $hkl \leq 333$; i.e., $(\sin\theta/\lambda) \leq 0.46$ Å^{-1}, and thus cannot be expected to provide information on the anharmonic term in the effective atomic potential or the nonrigid atomic thermal motion, which are expected to be non-negligible only for $(\sin\theta/\lambda) > 0.75$ Å^{-1}. In addition, while relativistic effects on the electronic wave functions are fairly small in germanium, they should be measurable with present day accuracies for $(\sin\theta/\lambda) > 1$ Å^{-1}. Thus, a high accuracy measurement of germanium structure factors in the range $0.45 \leq (\sin\theta/\lambda) \leq 1$ Å^{-1} appears to be most desirable.

We have undertaken such measurements, and the results are presented here. The measurement method is presented in the next section. The results obtained are presented in Sec. III along with a comparison with theory and a full discussion.

II. EXPERIMENTAL METHOD

The Laue case rocking curves of two thin perfect crystals exhibit pendelosung-type fine structure, the details of which depend very sensitively on the structure factor F_h of the reflecting plane.[18] Thus, by computer fitting the theoretical curve [Eq. (1) below] to the measured rocking curve it is possible to determine F_h accurately.[14,19,20]

The measured intensity as a function of the offset angle α of the crystals is given by[21]

$$I(\alpha) = I_0 \sum_{\sigma,\pi} \int I_R^{\sigma,\pi}(\theta) I_R^{\sigma,\pi}(\theta+\alpha)\, d\theta \tag{1}$$

where σ, π denote the polarizations of the radiation, and

$$\begin{aligned} I_R(\theta) = {} & [\exp(-\mu t/\cos\theta_B)/2(1+y^2)] \\ & \times \{\cosh[\mu t \epsilon (1+y^2)^{-1/2}/\cos\theta] \\ & - \cos[(2\pi t/\Delta_0)(1+y^2)^{1/2}]\} \,. \end{aligned} \tag{2}$$

Here μ, t, and θ_B are the linear absorption coefficient, the crystal thickness, and the Bragg angle, respectively, and ϵ is a slowly varying parameter of order unity.[14] y and Δ_0 are the angular parameter and the extinction length:[21]

$$\begin{aligned} y &= (\theta - \theta_B)\sin(2\theta_B)/C|x_{hr}| \,, \\ \Delta_0 &= \lambda \cos\theta_B / C|x_{hr}| \,, \end{aligned} \tag{3}$$

where θ is the angle of incidence, λ is the wavelength, and C is the polarization factor. x_{hr} is given by

$$x_{hr}=(r_e\lambda^2/\pi V)|F_h| \ , \tag{4}$$

where r_e is the classical electron radius, V is the unit cell volume, and F_h is the temperature-modified structure factor. Further details are given in Refs. 14 and 20.

Optimal measurements of the fine structure require that[11,14,20] $\mu t \le 1$ and $t/\Delta_0 > 1$. As μ decreases while Δ_0 increases with energy, these requirements impose opposing limitations on the wavelengths to be used in the measurements, as well as on the crystal thickness t. Furthermore, as germanium is rather fragile, practical considerations further restrict the crystal thickness to $t > 0.3$ mm. The variation with energy of Δ_0 and of t for a fixed μt is shown in Fig. 1. The dashed line indicates the $t = 0.3$-mm limit. It is clearly seen that the $\mu t < 1$ requirement restricts the usable energy range to $E > 40$ keV. At the lower end of this range all reflections $hhh \le 777$ also fulfill $t/\Delta_0 > 1$, as required. Increasing the energy will have the beneficial effect of reducing μt, but also undesirably reducing the ratio t/Δ_0 below the unity limit for high-order reflections. As the best compromise between these opposing requirements, as well as from practical reasons of intensity and availability, we chose to use the W $K\alpha_1$ ($E = 59.3$ keV) line from a fine focus (0.4×0.4 mm^2) industrial tungsten x-ray tube run off a 160-kV Pantak generator. To compensate for the increase in Δ_0 with energy, a nominal crystal thickness of 0.4 mm was chosen, thus observing both restrictions on t. At this high energy, the widths of the intrinsic reflection curves are extremely narrow. The 555 reflection, for example, is only 0.12 sec of arc wide. Alignment and stability problems thus clearly favor the monolithic design used in previous studies of very narrow rocking curves.[14,20,22] Thus a monolithic double-crystal diffractometer was employed for the measurements and is shown in Fig. 2. A rotation of one wafer relative to the other is done by bending the leaf sping cut between the wafers. This, in turn, is done by current-controlled magnetic interaction between a small permanent magnet attached to the block carrying one of the wafers and a small electromagnet attached to the bracket holding the device. Such a drive has been shown to be linear, smooth, repeatable and stable to better than 10^{-3} sec of arc.[14,20] The sharpness of the fine structure detected at the highest-order reflection measured, 777, attests to this as well. Further details on the design and properties of the monolithic diffractometer are given in Refs. 14 and 20.

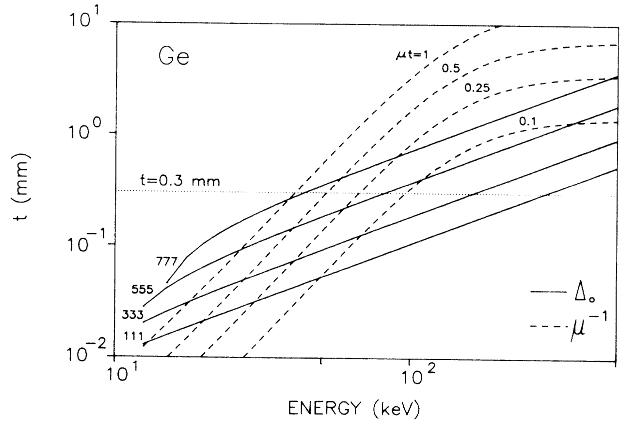

FIG. 1. Design parameters for thin crystal Laue-case rocking-curve measurements. The opposing requirements of $t/\Delta_0 > 1$ and $\mu t < 1$, where t, μ, and Δ_0 are the crystal thickness, the linear absorption coefficient, and the extinction length, respectively, clearly favor the use of high energies. For details see text.

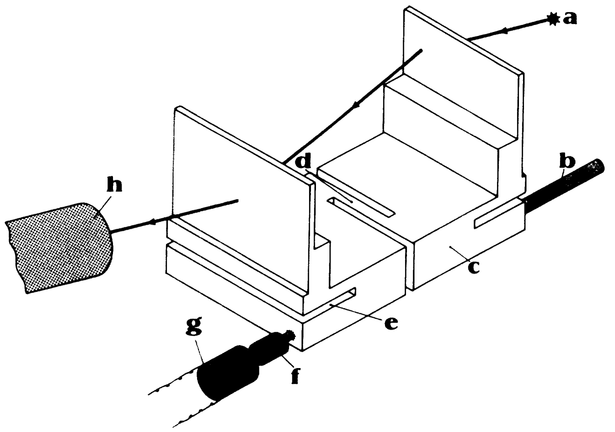

FIG. 2. Monolithic Laue diffractometer. (a) X-ray beam; (b) mounting post; (c) block; (d) leaf spring; (e) strain relief cut; (f) permanent magnet; (g) electromagnet; (h) detector. For details see text.

A simple passive thermal enclosure made of rubber foam on the inside and 3-mm-thick lead on the outside provided 0.1 °C temperature stability over 2 h, and ample vibration and radiation isolation. The small Bragg angles at the short wavelength used dictate a large (~ 2 cm) distance between the wafers to allow ample lateral displacement of the twice-reflected beam from the twice-transmitted one. 25-cm-long ground molybdenum parallels[23] were used to collimate the incident and twice-reflected beam. These, as well as the HPGe energy dispersive detector employed, provided adequate discrimination against spurious reflection and scattered radiation, both of which are serious problems at the short wavelength employed.

III. RESULTS AND DISCUSSION

A. Measured structure factors

Measurements were carried out on the same diffractometer for hhh ($h = 1,3,4,5,7$) reflections using the W $K\alpha_1$ line, $\lambda = 0.2097$ Å, and 6–10 curves were measured for each reflection. Although curves for the 888 and 999 reflection were also measured, intensity, signal-to-noise ratio, and wafer-thickness limitations did not allow an accurate determination of the corresponding structure factors. A single scan of the 333 reflection is shown in Fig. 3, along with the fitted curve, Eq. (1). Note the excellent fit. The residuals are randomly distributed and well within the statistical 2σ level of the data. The sharpness of the fine structure indicates the high stability of the diffractometer. Even at the much narrower high-

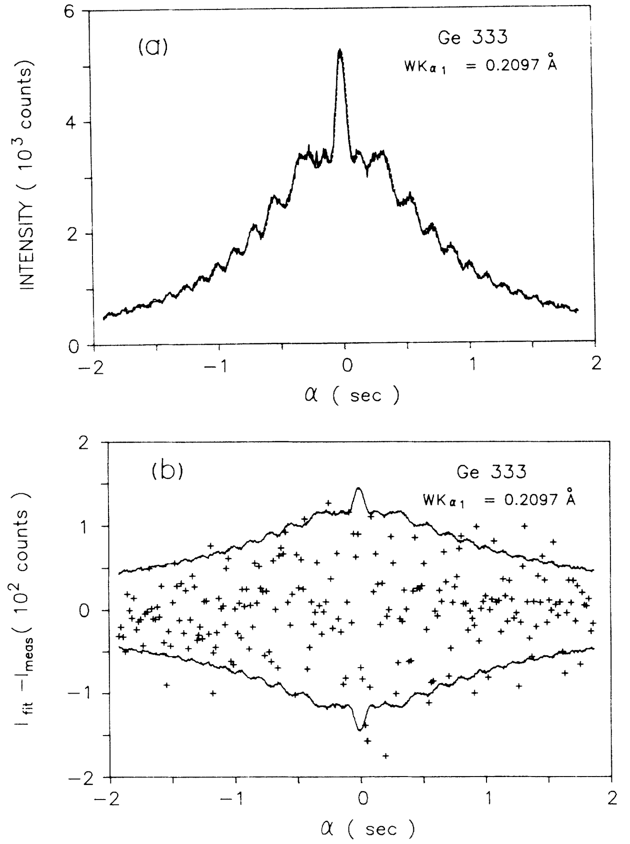

FIG. 3. The 333 rocking curve, (a) measured (——) and fitted (— — —). (b) Fit residuals (+) and the statistical $\pm 2\sigma$ levels (——) of the measured data. The excellent fit is indicated by almost all of the residuals being within the 2σ limits.

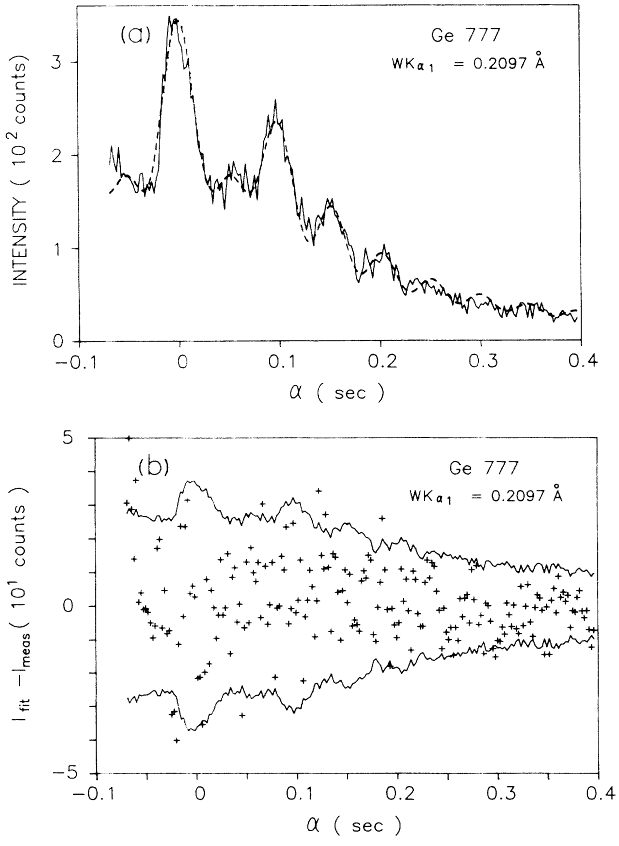

FIG. 4. Same as Fig. 2 for the 777 reflection in Ge. Note that in spite of the much narrower curve, the structure observed is sharp, demonstrating the high stability of the monolithic diffractometer.

order 777 reflection shown in Fig. 4, the features are sharp and the fit of Eq. (1) to the measured data is excellent. The structure factors $|F_m|$ obtained, adjusted[14] to 20 °C, are listed in Table I. The errors cited are the mean standard deviations from the mean of the values obtained from the fits done to the curves measured for each reflection. Note that all errors are $<0.25\%$.

To minimize the influence of strains, defects, and inhomogeneities on our results, the diffractometer was cut from a specially selected single-crystal boul, measured to be free from dislocations and lineages at both ends. Furthermore, a number of the rocking curves recorded for each reflection were measured with the beam illuminating different spots on the wafer. All such curves were found to be identical to within the statistical accuracy of the data, and no extra broadening could be detected. The fitted F values derived from these curves have a narrow distribution, as can be seen from the standard deviations given in Table I. We are, thus, confident that our results are free from strain effects, within the errors cited.

B. The dispersion correction

In order to compare the results of Table I with theory and previous measurements, it is necessary to correct for anomalous dispersion. Unfortunately, *measured* dispersion correction values f' are not available for germanium at the W $K\alpha_1$ wavelength. Moreover, several experimental studies[24] on Si, Ca, LiF, and other materials indicate that the widely used theoretical f' values of Cromer and Liberman[25] deviate significantly from the measured values. For high accuracy work on silicon, *measured* f values were proven[13] to be indispensible.

TABLE I. Measured structure factors F_m per atom for germanium. The variation in the last two digits due to the mean standard deviation in each value is given in brackets.

hkl	111	333	444	555	777
$\sin\theta/\lambda$ (Å^{-1})	0.1531	0.4592	0.6122	0.7653	1.0714
F_m (electrons)	27.638(52)	15.470(15)	11.056(24)	7.765(17)	3.981(10)

Using the very detailed analysis of Gerward *et al.*[26] of f' for silicon, we find from Table I in Ref. 26 that the best agreement between theory and experiment is obtained for the average between the relativistic Cromer-Liberman value f'_{CL} and that of the real part of f' calculated over the positive energy states only, f_r^+. Employing the same practice for germanium, we obtain the f' values listed in Table II. Here f'_{CL} values were calculated using the Cromer-Liberman program adapted by Templeton[27] for IBM-PC computers. The f_r^+ values were taken from Table II of Ref. 26, and for W $K\alpha_1$ from Fig. 3(b) there. Admittedly, the procedure employed here has no theoretical justification. However, the values obtained are in good agreement with those previously used in the literature for $K\alpha_1$ radiations of Cu, Mo, and Ag. This, as well as the excellent results obtained by this method for silicon, induces additional confidence in the value of $f'_{\mathrm{W}\,K\alpha_1}=0.090$ electrons, calculated for our wavelength. The consequences of possible errors in this value are discussed below.

C. Corrected F_h values, and the Debye parameter B

Using now the f' value of Table II and the nuclear scattering correction $f_N=0.0077$, we calculate the energy-independent F_c value from

$$F_c=F_M-(f'_{\mathrm{W}\,K\alpha_1}+f_N)\exp[-B(\sin\theta/\lambda)^2]\ , \tag{5}$$

using first the Debye parameter $B=0.567$ Å^2 of Batterman and Chipman.[33] Excluding F_{111} on grounds of non-negligible bonding contributions, a new value for B was calculated by a linear fit of $\ln(F_c/f)$ versus $(\sin\theta/\lambda)^2$, using, in turn,[34] f_{RHF} and [35] f_{HF} from Table III and requiring the fit to pass through the origin. The new B was used to calculate F_c using Eq. (5) and the fit repeated. Two iterations were sufficient to reach convergence, and we obtained

$$\begin{aligned} B_{\mathrm{RHF}}&=(0.5661\pm0.0026)\ \text{Å}^2\ ,\\ B_{\mathrm{HF}}&=(0.5548\pm0.0045)\ \text{Å}^2\ . \end{aligned} \tag{6}$$

These values, and in particular B_{RHF}, are in excellent agreement with those of Batterman and Chipman,[33] $B=(0.567\pm0.01)$ Å^2, and Matsushita and Kohra,[16] $B=0.560$ Å^2, though less with $B=0.610$ Å^2 of the same authors. It should be noted that if the fit is not required to pass through the origin, the y intercept obtained is (-0.0032 ± 0.0034), i.e., still zero, within error. The temperature-corrected structure factors f_m obtained from $f_m=F_c\exp[B(\sin\theta/\lambda)^2]$ using the B's above are listed in Table III along with previous measurements, free-atom structure factors using relativistic[34] (RHF) and nonrelativistic[2] (HF) wave functions, and a few theoretical predictions. Excellent agreement is obtained with the values of Matsushita and Kohra[16] and one of the f_m values of Batterman and Patel.[31] The agreement with other measurements is slightly less good, but still within reason. Note, however, that all previous high-accuracy measurements are restricted to 111 and 333 only. The low-accuracy values of DeMarco and Weiss[30] agree with ours except for the 555 reflection. The theoretical predictions seem to consistently underestimate f_{111} and f_{333}, indicating perhaps that bonding effects were not fully accounted for.

We have also explored the influence of an incorrectly chosen f' on our results by repeating the analysis detailed above for values of f' increasingly deviating from the nominal $f'=0.09$. Previous analyses of silicon data[14] indicate that for energies far removed from the K edge, the results are relatively insensitive to the exact value of f'. The same results were found here. For example, a 50% increase in f', i.e., $f'=0.135$, yields $B_{\mathrm{RHF}}=(0.5719\pm0.0027)$ Å^2, which is within ~1.1 SD only from the value given in Eq. (6), where SD is the combined mean standard deviation in the two values. Moreover, the values of f_m obtained vary from those given in Table III by less than one half of the experimental errors cited, σ, for all but f_{333}, which deviates by slightly less than 1σ. Even for a 100% deviation in f' we find a deviation of $<1\sigma$ for f_{444}, f_{555}, and f_{777}, $<2\sigma$ for f_{111}, and $\sim3\sigma$ for f_{333}, and a reasonable value of $B_{\mathrm{RHF}}=(0.5778\pm0.0026)$ Å^2.

We conclude therefore that even for the present high-accuracy data, the analysis and conclusions presented above are fairly insensitive to the exact value of f'. While an accurate determination of f' would be very desirable for its own sake, such a datum is likely to be mandatory only for the analysis of data fivefold–tenfold more accurate than obtainable at present.

TABLE II. The dispersion correction f' for germanium. The method of calculation is given in the text. Note the close agreement of f' with previous values for the first three wavelengths.

$K\alpha_1$	λ (Å)	f_r^+[a]	f'_{CL}	f'	Previous values		
Cu	1.5406	−0.980	−1.163	−1.07	−1.04[b]	−1.31[c]	
Mo	0.7093	0.270	0.080	0.18	0.24[d]	0.2[e]	
Ag	0.5594	0.410	0.227	0.32	0.3[f]	0.36[c]	0.36[g]
W	0.2097	0.173	0.006	0.09			

[a] Reference 26.

[b] Reference 28.

[c] Reference 16.

[d] Reference 29.

[e] Reference 30.

[f] Reference 31.

[g] Reference 32.

TABLE III. Atomic scattering amplitudes f_m corrected for dispersion, nuclear scattering, and the Debye-Waller factor. Previous measurements, as well as theoretical predictions, are also listed.

	Present work		Experimental					Free atom		Theoretical	
hkl	RHF	HF	MK[a]	TS[b]	BP[c]	DMW[d]	*J*[e]	RHF[f]	HF[g]	WK[h]	YC[i]
111	27.908(53)	27.901	27.880(60)	27.230(90)	27.000(200) 28.290(250)	27.550(200)	27.520(120) 27.550(120)	27.380	27.351	27.46	27.47
333	17.333(17)	17.291	17.330(100)			17.520(200)		17.339	17.305	17.22	17.16
444	13.570(30)	13.513				13.500(150)		13.509	13.441		
555	10.719(24)	10.647				10.230(150)		10.704	10.590		
777	7.526(19)	7.428				7.23(150)		7.542	7.460		

[a] Reference 16.
[b] Reference 17.
[c] Reference 31.
[d] Reference 32.
[e] Reference 28.
[f] Reference 34.
[g] Reference 2.
[h] Reference 39.
[i] Reference 6.

D. The anharmonic temperature factors and nonrigid atomic vibrations

The effective one-particle anharmonic potential is, to the lowest order,[1,36]

$$V=\tfrac{1}{2}\alpha(x^2+y^2+z^2)+\beta xyz \ , \qquad (7)$$

which yields[1,12] the following harmonic and anharmonic temperature factors, respectively:

$$T_c=\exp[-B(\sin\theta/\lambda)^2]$$
$$=\exp[-(8\pi^2 k_B T/\alpha)(\sin\theta/\lambda)^2] \qquad (8)$$

and

$$T_a=T_c(k_B T)^2[8\pi^3\beta/(a_0\alpha)^3]hkl \ . \qquad (9)$$

Here k_B is the Boltzmann constant, T is the temperature, $a_0=5.658$ Å is the lattice spacing of Ge, and *hkl* are the Miller indices of the reflection under consideration. From our B_{RHF} of Eq. (5) we obtain $\alpha=(5.646\pm0.026)\times10^{-12}$ erg/Å^2, in excellent agreement with $\alpha=(5.64\pm0.1)\times10^{-12}$ erg/Å^2 calculated by us for 20 °C from the germanium Debye temperature measured by Batterman and Chipman.[33] Taking now[35] $\beta=2.035\times10^{-12}$ erg/Å^3 we obtain

$$T_a/T_c=2.54\times10^{-5}hkl \ \text{ at } 20\,^\circ\mathrm{C} \ . \qquad (10)$$

This value is about 3 times the upper limit on the same quantity obtained by us[14] for silicon. Dawson's theory[2,12,14] shows that the ratio given in Eq. (10) should cause a relative *decrease* of $T_a/T_c=3.2\times10^{-3}$ in f_{555}, and a relative *increase* of $T_a/T_c=8.7\times10^{-3}$ in f_{777} compared with the theoretical free-atom harmonic-potential f_{RHF} listed in Table I. In Fig. 5 we plot the relative difference between f_m and the theoretical f_{RHF} and f_{HF} for our data, excluding f_{111}, which includes an appreciable bonding contribution. As can be seen, f_{555} and f_{777} do not deviate, within error, from the free-atom RHF values. If at all, the measured values seem to deviate in the opposite direction, in particular relative to the HF values. Our data, therefore, seem to indicate that β is smaller than that measured by Batterman and coworkers[35,37,38] by perhaps a factor of 2–3. This is in keeping with silicon, where a factor of 3–4 was found.[12,14,22] Note, however, that another explanation is also possible. Our conclusion on the magnitude of β rests mainly on the measured value of f_{777}, as the deviation in f_{555} is too close to the measurement uncertainty. If the nonrigid thermal motion effect, found in silicon,[14,22] occurs here as well with roughly the same magnitude, it will result in a *downshift* of about 1% in f_{777} and practically none in f_{555}. Thus, it is possible that the agreement of the measured f_{777} with the harmonic $f_{\mathrm{RHF,HF}}$ value results from a cancellation of the 0.9% upshift of f_{777} due to β by the 1% downshift due to the nonrigid thermal motion, and no contradiction between the results of Batterman and co-workers[35,37,38] and our data occurs. To resolve this question, the structure factors of higher-order reflections, where the two effects are of unequal magnitude, should be measured to an accuracy commensurate with the present results. Reflections where $hkl=0$, and hence $T_a/T_c=0$, should, in particular, be very useful in this respect.

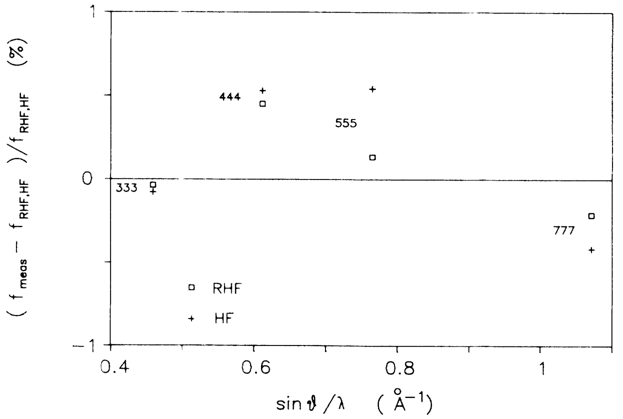

FIG. 5. Relative difference between measured (f_m) and free-atom theoretical ($f_{\mathrm{RHF,HF}}$) scattering amplitude. Note that the expected ~1% upward shift of f_{777}, predicted to result from the anharmonic term in the effective single-atom potential, is not observed.

IV. CONCLUSIONS

We present here measured values of structure factors of germanium in the range of $0.15 \leq \sin\theta/\lambda \leq 1.07$ Å^{-1}, and an accuracy $\leq 0.25\%$. A fourfold increase in accuracy is obtained for the value of the Debye parameter B, derived from our data over previous results.[33] No support is found in the data for an anharmonic force constant β larger than about half of that measured previously,[35,37,38] nor for a nonrigid thermal motion of the atom, which was observed in silicon.[14,22] These negative results may, however, result from a cancellation of these effects for the only measured reflection, 777, where they should be appreciably larger than the experimental uncertainty. Clearly, similar high-accuracy measurements are indicated for reflections in the range $\sin\theta/\lambda \geq 1.07$ Å^{-1} to unambiguously determine the relative importance and magnitude of these effects. Finally, while in Fig. 5 f_{RHF} seems to yield better agreement than f_{HF} with all measured values, a real assessment of the relativistic contribution to f can only be made at higher $\sin\theta/\lambda$ values, where this contribution is well above the 0.25% uncertainty level.

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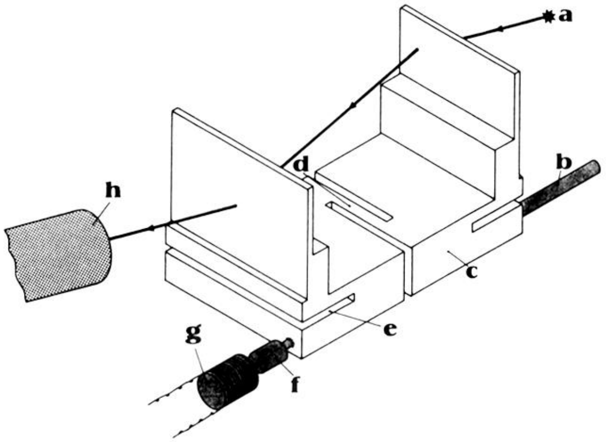

FIG. 2. Monolithic Laue diffractometer. (a) X-ray beam; (b) mounting post; (c) block; (d) leaf spring; (e) strain relief cut; (f) permanent magnet; (g) electromagnet; (h) detector. For details see text.