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Temperature dependence of planar channeling radiation

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Peak energies and linewidths of 54-MeV electron planar channeling radiation from a silicon crystal have been measured as a function of temperature. Our measured peak energies are compared with our theoretical calculations to obtain a Debye temperature for silicon of 495±10 K. This value is appreciably lower than the value of 543 K obtained from an x-ray diffraction measurement, but is in excellent agreement with the value of 500 K obtained recently from a measurement of axial channeling radiation.

In this paper we report measurements of 54-MeV electron planar channeling radiation spectra as a function of temperature down to liquid-nitrogen temperature, for a silicon crystal. For electron channeling, the thermal vibration of the atoms, which causes transitions between bound eigenstates as well as dechanneling, is the primary contributor to the linewidth.[1] At lower temperature the linewidth is reduced, since the thermal vibration of the atoms decreases with temperature. Another effect of cooling is to shift the spectral lines to higher frequencies. The potential well for a fixed atom is deeper than the corresponding well for a vibrating atom, and in the former case there is greater separation between the energy eigenvalues. Figure 1 shows the silicon (110) planar potential at 80 and 293 K.

The measurements reported here were done with 54-MeV electrons from the Lawrence Livermore National Laboratory Electron-Positron Linear Accelerator. Details of the experimental setup can be found in Ref. 1. In the present experiment, a 19-μm-thick, $\langle 100 \rangle$ axis silicon crystal was mounted on a copper cold finger which was clamped to a small refrigerator.[2] The whole system was mounted in our goniometer, in which heat exchange with the surroundings was by radiation only and was minimal.

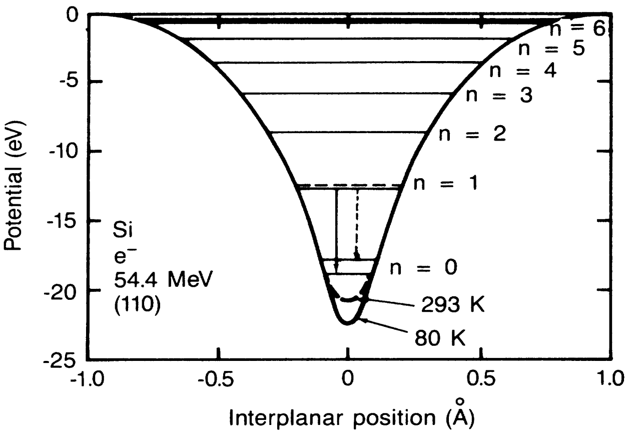

FIG. 1. Potentials and eigenvalues for the (110) plane in silicon for two different temperatures, 80 and 293 K. The eigenvalues are calculated for 54.4-MeV ($\gamma = 107.5$) electrons. In the potential calculation, a Debye temperature of 495 K was used. Notice the large shift of the $n = 0$ level with temperature. For the $n \geq 2$ levels, the changes of eigenvalues with temperature is very small and cannot be observed in this figure.

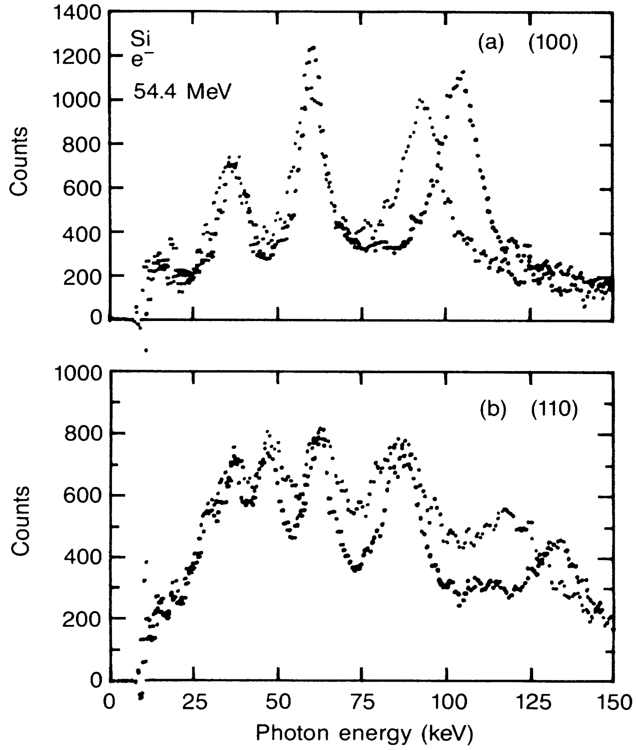

FIG. 2. Channeling-radiation spectra for 54.4-MeV electrons at room temperature and at low temperature. (a) Silicon (100) spectra at 5 °C and −190 °C; (b) silicon (110) spectra at 7 °C and −180 °C. The large dots represent the low-temperature data and the small dots represent the room-temperature data.

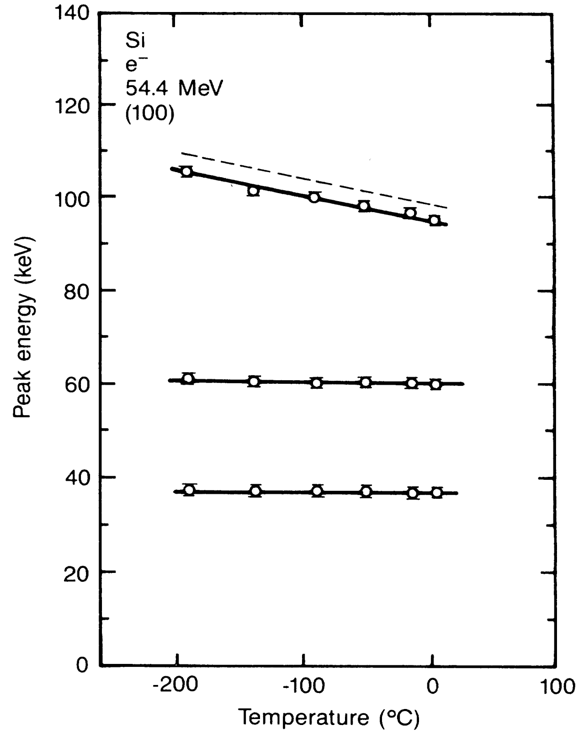

FIG. 3. Channeling-radiation peak energies from 54.4-MeV electrons for the (100) plane in silicon as a function of temperature. The circles represent the measured values; the solid line is the result of the calculation using a Debye temperature of 495 K. The dashed line shows the theoretical 1 ⟶ 0 transition energy calculated using a Debye temperature of 543 K.

The crystal temperature was monitored by two thermometers: one was built into the refrigerator and the other one was attached to the silicon crystal. Both yielded temperature readings within 1 K of each other, showing that the thermal load was well within the capacity of the refrigerator.

Figure 2 shows the 54-MeV electron channeling-radiation spectra from the (100) and (110) planes at room temperature and at low temperature. The heavy dots are the low-temperature data [−190 °C for the (100) plane and −180 °C are the (110) plane], and the light dots are the room-temperature data. One can observe a large upshift of 1 ⟶ 0 transition energy, along with some line narrowing, for the low-temperature case.

Figures 3 and 4 show the measured channeling-radiation peak energies as a function of temperature, together with values calculated from the many-beam formalism, using a thermal-vibration amplitude corresponding to a Debye temperature of 495 K. Also, theoretical values of 1 ⟶ 0 transition energies calculated using a Debye Temperature of 543 K (Ref. 3) as shown in dashed lines.

In the comparison, we used a two-step procedure. Since transitions between states having $n \geq 1$ are not affected significantly by the change of thermal-vibration amplitude, we have a good way of checking whether the experiments were done properly. For the 2 ⟶ 1 and higher tran-

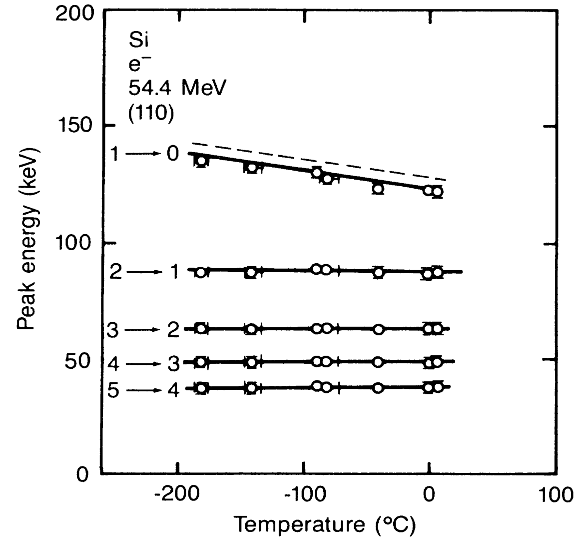

FIG. 4. Channeling-radiation peak energies from 54.4-MeV electrons for the (110) plane in silicon as a function of temperature. The circles represent the measured values; the solid line is the result of the calculation using a Debye temperature of 495 K. The dashed line shows the theoretical 1 ⟶ 0 transition energy calculated using a Debye temperature of 543 K.

TABLE I. Channeling-radiation peak energies as a function of temperature for 54.4-MeV electrons channeled along the (100) planes of silicon.

	Peak energies (keV)						
	Measured						
Transition	5 °C	−13 °C	−50 °C	−89 °C	−137 °C	−190 °C	Calculated[a]
1→0	94.0±1	96.5±1	98.1±1	99.7±1	101.2 ±0.8	105.4 ±0.8	97.8 110.4
2→1	59.9 ±0.8	60.6 ±0.8	60.6 ±0.8	60.4 ±0.6	60.5 ±0.8	61.1 ±0.6	62.8 63.6
3→2	36.9 ±1.0	36.8 ±1.0	37.2 ±1.2	37.4 ±1.0	37.4 ±1.0	37.2 ±1.0	37.8 37.7

[a] Two values are for two extreme temperatures; the first one is for 5 °C and the second for −190 °C. A Debye temperature of 495 K is used in calculation.

sitions for both planes, i.e., (100) and (110), we note from Table I and Table II that the theoretical values are 4% higher than the experimental results. Therefore, all of the calculated peak energies plotted in Figs. 3 and 4 are 4% lower than the original calculated values. By this procedure, we correct (presumably) for any small error in the experimental alignment or energy calibration.

With this 4% modification of the calculated values, all of the calculated values except those for the 1→0 transition match well with the experimental results. By varying the Debye temperature (in the form of the thermal-vibration amplitude) we fitted the calculated 1→0 transition energies to the observed ones. Best fits were obtained for a Debye temperature 495±10 K for both the (100) and the (110) plane data. This value is close to the values of 499 K calculated by Dolling and Cowley using the shell model[4] and 500 K measured by Andersen *et al.* from axial channeling-radiation data.[5] However, it is somewhat lower than the value of 526 K calculated by Nielson and Weber using a bond-charge model.[6] Also, it is substantially lower than the value of 543 K obtained earlier by Batterman and Chipman from their x-ray diffraction data.[3] A value of 543 K for Debye temperature gives the dashed lines in Figs. 3 and 4, which lie well outside the experimental uncertainty.

A possible source of error in our determination of the Debye temperature may be inherent in the use of an average crystal potential. In calculating peak energies in planar channeling radiation, one starts with the planar-average potential. Assuming a Gaussian distribution of atoms, one can get the final form of the potential. From the potential one then can calculate the radiation peak energies[7,8] easily and conveniently. This procedure gives excellent agreement between the measured and calculated transition energies for diamond,[1] Ge,[9] and GaAs.[10] However, the rigorous approach is to solve the Schrödinger equation for the frozen lattice sites at different times and to average the peak energies subsequently. This method is quite complicated, but should be looked into to see whether it yields a different value.

Our measured linewidths are compared with our calculated values in Figs. 5 and 6. For both planes the agreement is reasonably good. In the calculation three line-broadening mechanisms were included: Bloch-wave broadening, Doppler broadening due to multiple scattering, the lifetime broadening. (Other line-broadening ef-

TABLE II. Channeling-radiation peak energies as a function of temperature for 54.4-MeV electrons channeled along the (110) planes of silicon.

	Peak energies (keV)							
	Measured							
Transitions	7 °C	0 °C	−40 °C	−80 °C	−89 °C	−104 °C	−180 °C	Calculated[a]
1→0	121.4 ±1.5	122.0 ±1.2	122.8 ±2.0	127.0 ±2.0	129.5 ±1.5	131.9 ±1.5	134.3 ±1.5	125.4 142.3
2→1	87.3 ±1.2	86.6 ±1.0	86.8 ±1.0	88.2 ±1.0	88.3 ±1.0	87.5 ±0.8	87.1 ±0.8	90.3 93.4
3→2	63.1 ±1.0	62.6 ±1.0	61.9 ±0.8	62.9 ±0.8	63.3 ±0.8	62.2 ±0.8	62.8 ±0.8	65.4 65.0
4→3	47.8 ±1.0	48.1 ±0.8	48.1 ±0.8	48.5 ±0.8	48.6 ±0.8	48.4 ±0.6	48.0 ±0.8	50.0 50.4
5→4	37.6 ±1.0	37.4 ±1.0	36.6 ±1.0	37.1 ±0.8	37.6 ±0.6	36.8 ±0.8	36.9 ±0.6	38.8 38.7

[a] Two values are for two extreme temperatures. The first one is for 7 °C and the second for −180 °C. 495 K is the Debye temperature used in calculation.

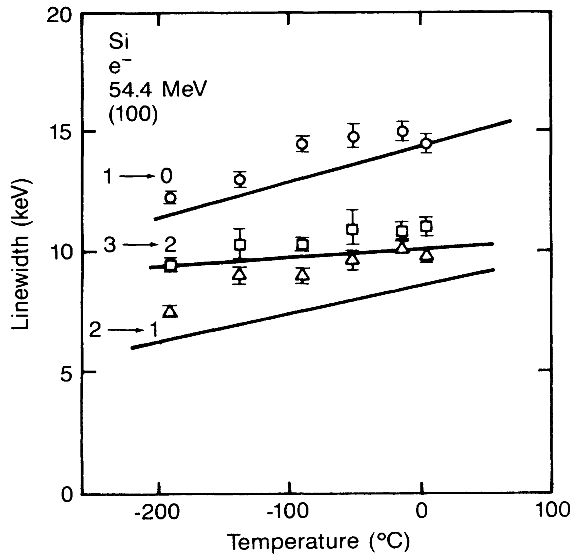

FIG. 5. Measured and calculated channeling-radiation linewidths as a function of temperature, for 54.4-MeV electrons channeled along the (100) planes of silicon. In the calculation, a Debye temperature of 495 K was used. Squares are for $3\rightarrow2$ transitions and triangles are for $2\rightarrow1$ transitions.

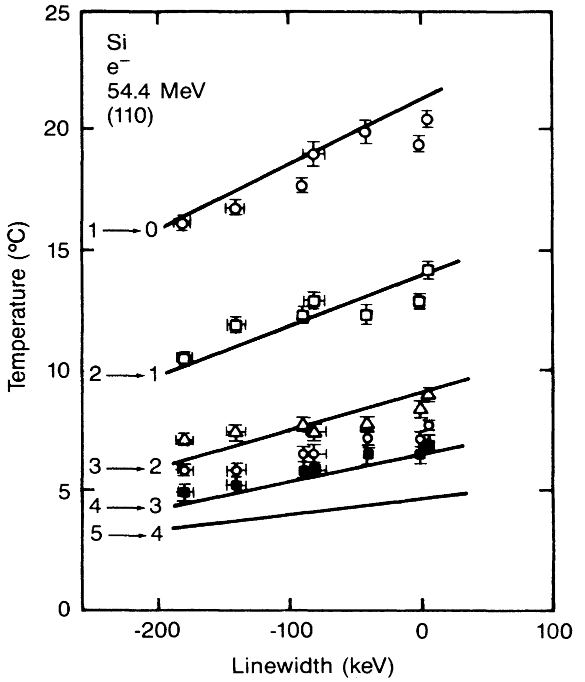

FIG. 6. Measured and calculated channeling-radiation linewidths as a function of temperature, for 54.4-MeV electrons channeled along the (110) planes in silicon. In the calculation, a Debye temperature of 495 K was used.

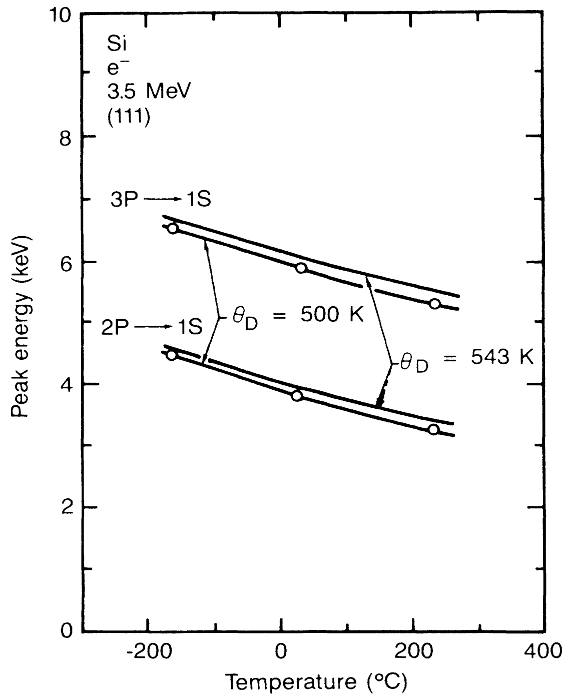

FIG. 7. Measured and calculated $3P\rightarrow1S$ and $2P\rightarrow1S$ transitions of 3.5-MeV electron axial channeling radiation for ⟨111⟩ axis of silicon as a function of temperature (experimental data from Ref. 5). The solid lines were calculated using two different Debye temperatures, for comparison.

fects that we have considered are minor and do not affect our calculation in any significant way.[1]) The values for the linewidths from these three effects were added in quadrature to produce the values shown in Figs. 5 and 6. Generally, one can expect that the linewidth would broaden as the temperature increases, due to the increase of multiple scattering. The other two effects considered here do not vary as the temperature changes.

Figure 7 shows the experimental values of Ref. 5 compared with two calculated values. In this case, the assumed Debye temperature are 543 and 500 K, the latter value corresponding to the best fit to their data. Both results indicate that 543 K is too high.

In conclusion, we observe an energy upshift and a linewidth narrowing of the peaks in the spectra for electron planar channeling radiation from silicon as the crystal temperature is lowered. The Debye temperature which corresponds to the best fit to our data is 495±10 K. This is in agreement with the theoretical value of Ref. 3 and the experimental value of Ref. 4, but not with the x-ray diffraction value of Ref. 7. Our measured linewidths generally fit well with calculated values for the Debye temperature of 495 K.

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