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INELASTIC X-RAY SCATTERING FROM 6H-SiC

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We have studied electronic excitations in 6H-SiC using inelastic x-ray scattering. Inelastic scattering spectra were measured at momentum transfers ranging from 0.47 \AA^{-1} to 2.00 \AA^{-1} along the c-axis in the hexagonal lattice, i.e., along [00·1], and from 0.67 \AA^{-1} to 2.00 \AA^{-1} along the a-axis, i.e., along [10·0]. Comparison of the two sets of data reveals an orientation dependence of the spectra, except for a characteristic peak at 22-23 eV that occurs for both directions at low Q. This peak has also been observed in electron energy loss spectroscopy studies and is identified as a bulk plasmon. The orientation dependence of the other spectral features is indicative of band structure effects. These data were obtained using a Ge(444) analyzer in a near backscattering geometry.

I. Introduction

Interest in SiC stems not only from its potential use in devices (e.g., blue LEDs and ultraviolet photodiodes), but also from fundamental interest in the application of local-density-approximation (LDA) calculations to this material [1,2]. Band gaps for semiconductors and insulators obtained from such calculations have been consistently underestimated by (30-50%) compared with experiment [2]. SiC has attractive electronic, optical and thermal properties for use in practical devices, and a wide range of polytypes exists for which comparisons to theoretical results can be made.

Inelastic x-ray scattering (IXS) is a useful probe of a wide variety of electronic excitations [3]. Compton scattering is a well known type of IXS that is widely used to determine electron momentum distributions. With the advent of modern synchrotron sources, other types of IXS have become accessible and have been used to yield information not only on single particle and collective excitations of electrons but also on the lattice dynamics of solids. To achieve spectra that are useful for these purposes, one requires a resolution considerably higher than is typical for Compton scattering experiments. With a band pass ranging from 0.1 to 1 eV, one can study both valence band and conduction band electrons. The same energy resolution is also important for studies of collective excitations, e.g., plasmons. Electron energy loss spectroscopy (EELS) is widely used to provide information on collective electronic excitations but has the drawback that multiple scattering effects at high momentum transfers complicate the interpretation of the measurements. Because cross sections are very small, IXS measurements are much less susceptible to multiple scattering complications and are consequently more amenable to theoretical modeling. Furthermore, hard x-rays do not require the use of ultrahigh vacuum conditions, and bulk sampling is guaranteed.

II. Experimental Details

The 6H-SiC crystal had a large facet oriented along [00-1], and we positioned the sample so that the momentum transfer, Q , was either along this direction, i.e., along the c -axis of the hexagonal structure or perpendicular to this direction, i.e., along [10-0], the a -axis. Electron energy loss studies of the SiC crystal have also been made, and the present data are in agreement for the plasmon energy [4]. The IXS spectra were measured at beamline X21 at the National Synchrotron Light Source. This beamline has a wiggler as a source and delivers 2×10^{11} photons per sec in a bandwidth slightly less than 1 eV [5]. Crystal analyzers of increased collection efficiency have recently been constructed and were used for the present studies. We used a Ge (111) oriented analyzer set for the (444) reflection at 7.6 keV [6]. The Bragg angle was set in the range 86° to 87° . We used a NaI scintillation counter for collecting the scattered photons.

III. Results and Discussion

The IXS spectra we obtained are shown in Fig. 1. Spectra for momentum transfers ranging from 0.47 \AA^{-1} to 2.00 \AA^{-1} are shown. The spectra were normalized using the sum rule,

$$\int S(Q, \omega) \omega d\omega = \pi Q^2 / 2m.$$

Here $S(Q, \omega)$ is the dynamical structure factor for inelastic scattering at an energy loss denoted as $\hbar\omega$.

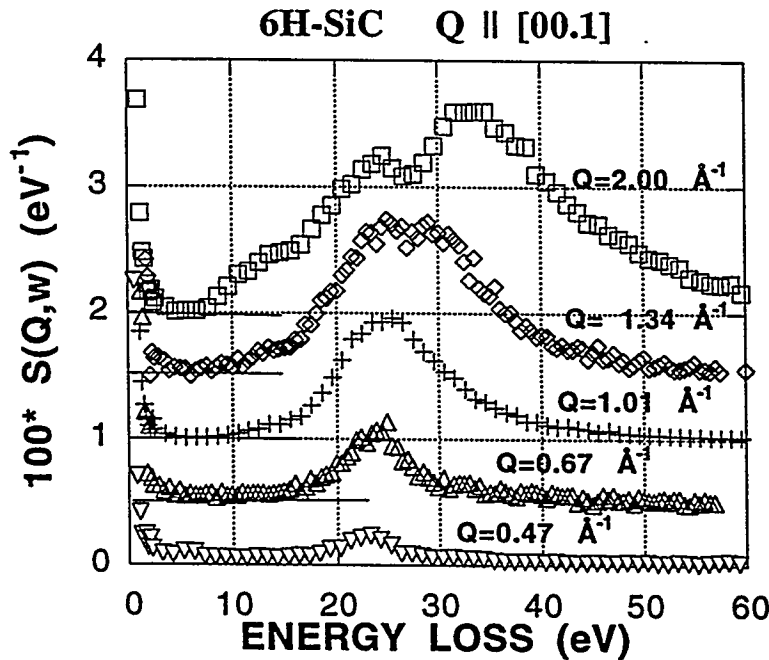


Fig.1 Inelastic x-ray scattering spectra for 6H-SiC for momentum transfers along the c -axis. The data are offset by 0, 0.5, 1.0, 1.5, and 2.0 ordinate units, respectively, for increasing Q .

In the free electron case and for Q below a critical value, Q_c , only intraband and plasmon excitations are allowed by energy and momentum conservation during the scattering process [7,8]. For SiC this value is given by $Q_c = 1.08 \text{ \AA}^{-1}$. This value for Q_c was obtained by invoking a free electron description for the 48 valence electrons in the large unit cell of 6H-SiC. That this description has at least partial validity is suggested [8] by the fact that the observed plasmon energy (22 -23 eV) is much larger than the band gap energy (3-5 eV). For Q values above Q_c , plasmons can decay to electron-hole pairs. Corrections to this free electron scheme arise if the periodicity of the crystalline lattice (i.e., the band structure) is also included.

The data shown in Fig. 1 reveal an overall qualitative agreement with the above description. A single peak remains in the spectra for the three Q s below 1.08 \AA^{-1} , and we identify this peak as the bulk plasmon. The dispersion of this peak is shown in Fig. 2 and follows a Q^2 dependence below Q_c . This behavior is similar to that found for simple alkali metals [8].

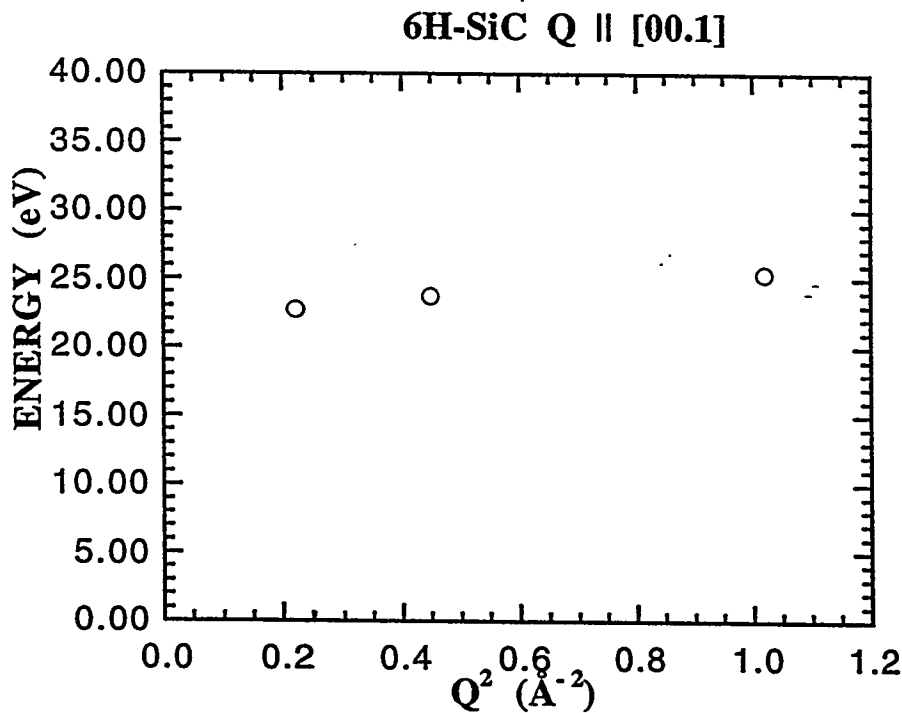


Fig. 2 Dispersion of the plasmon for 6H-SiC.

Spectra for $Q > Q_c$ have been of interest in the context of the many-body physics of the electron gas [9]. Recent calculations for Al [10] have found that, contrary to previous expectations, the data have a significant orientational dependence. We have also obtained IXS spectra for 6H-SiC with Q perpendicular to the c-axis. These data are for Q along [10·0], i.e., along the a axis, and are shown in Fig.3. A clear difference between the data in Figs. 1 and 3 is evident.

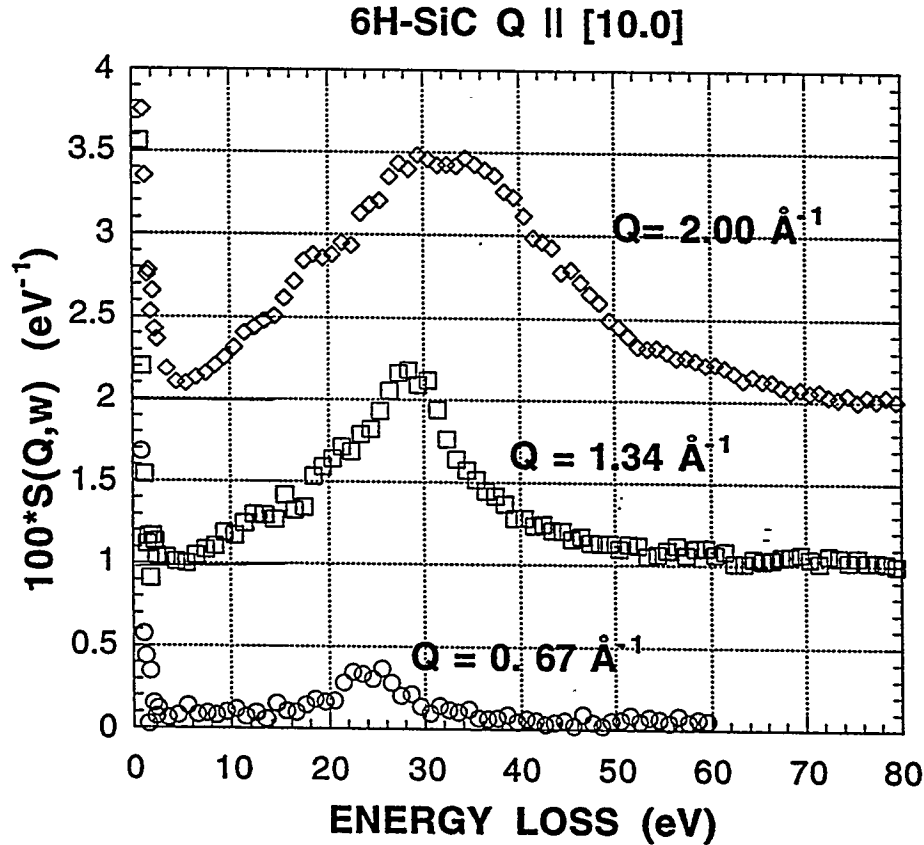


Fig. 3 . IXS data for momentum transfers along the a-axis. The data are offset by 0, 1 and 2 ordinate units, respectively, for increasing Q .

IV. Theoretical Comparisons

Calculations of the full momentum and frequency dependent dielectric constant can be made using local-density-approximation (LDA) calculations . These calculations also generate band structures. Such calculations can be compared to our data by means of the relationship,

$$S(Q, \omega) = \frac{\pi Q^2}{4\pi^2 N} \text{Im} \left(\frac{-1}{\epsilon(Q, \omega)} \right),$$

which is a form of the fluctuation-dissipation theorem [9]. The above data are expected to provide new insights into the means required to improve agreement between calculated band structures and data. Such comparisons are currently in progress [11].

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