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High-pressure system for Compton scattering experiments

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High-pressure apparatus for Compton scattering experiments has been developed to study the momentum distribution of conduction electrons in metals and alloys at high pressure. This apparatus was applied to observe the Compton profile of metallic Li under pressure. It was found that the Compton profile at high pressure could be obtained within several hours by using this apparatus and synchrotron radiation. The result on the pressure dependence of the Fermi momentum of Li obtained here is in good agreement with that predicted from the free-electron model.

Keywords: Compton scattering; high pressure.

1. Introduction

The observation of the Fermi surface or the momentum distribution of conduction electrons is most important to understand the electronic structure of metals and alloys (MA) because almost all the physical properties of MA are dominated by the behavior of conduction electrons. Compton scattering is well known to be a good technique to obtain the momentum distribution of conduction electrons (see Williams, 1977). The greatest difficulty in performing Compton scattering experiments is that one needs a strong X-ray source. It takes a long time to obtain a Compton profile when a conventional X- or γ-ray source is used. But recently it has become possible to use extremely intense X-rays from a synchrotron radiation (SR) source. Moreover, high pressure is also a good tool to investigate the electronic structure of MA since many electronic or structural phase transitions can be observed by applying pressure (Thompson & Lawrence, 1994). If these two techniques are combined, a large amount of useful information can be obtained to provide a deep insight into the electronic structure and mechanism of the phase transitions of MA. However, there have been few reports studying the momentum distributions of conduction electrons of MA under high pressure until now because of a lack of an intense X-ray source and technical difficulties in using high pressure (Oomi & Itoh, 1993; Oomi *et al.*, 1996). In the present paper we report the construction and use of high-pressure apparatus for Compton scattering measurements using SR.

2. Experimental methods

2.1. *High-pressure apparatus*

Fig. 1 shows a cross section of the present high-pressure apparatus developed for Compton scattering measurements. The high pressure was generated by using Bridgman-type sintered diamond anvils having faces of 3 mm in diameter. The pressure was applied by using a hydraulic press and clamped by using upper and lower driving screws (2 and 10 in Fig. 1). After clamping, the high-pressure apparatus was centered in the optical system, using an *XYZ* stage. The collimator was made of tungsten carbide and had a diameter of 0.2 mm. The optical system will be described in detail below. A beryllium disk (0.5 mm in thickness) was used as a gasket because it is transparent to X-rays. Before using the gasket, it was annealed at 773 K for 3 h to obtain good ductility. Compton scattering measurements were carried out by using a monochromated 59.34 keV X-ray beam from a multipole wiggler (Yamamoto *et al.*, 1989). The angle to observe the Compton scattered X-rays was 90°.

Polycrystalline Li was used as a sample because the contribution from the core electrons to the Compton profile is small. The Li sample, which is easily oxidized in air, was placed carefully in a small hole (0.5 mm in diameter), drilled in the center of the Be gasket, without any pressure medium.

2.2. *Optical system for Compton scattering measurements*

Fig. 2 shows a schematic diagram of the optical system used for the present Compton scattering measurements. The measurements were carried out at the AR NE-1 station of the Accumulation Ring Source at KEK, Tsukuba, Japan. The X-rays passing through the ion chamber were scattered by the Li metal sample

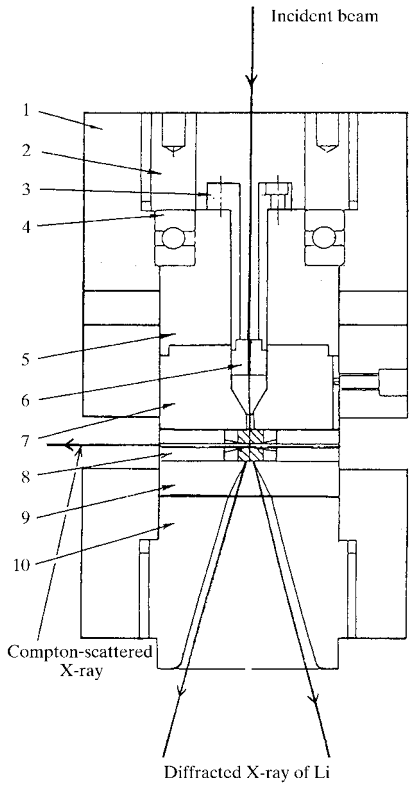

Figure 1
Cross section of the high-pressure apparatus for Compton scattering: (1) body, (2) driving screw, (3) collimator holder, (4) bearing, (5) piston, (6) collimator, (7) guide ring, (8) anvils, (9) spacer and (10) driving screw.

held in the high pressure cell at an angle of 90°. The scattered photons were detected by means of a solid-state detector.

In the present work the pressure inside the cell was determined by using the equation of state of Li (Olinger & Shaner, 1983). Measurement of the lattice constant of Li was performed simultaneously by using an imaging plate, which was placed at the back of high-pressure apparatus as is shown in Fig. 2. Typically it took about 3–5 h to accumulate a photon signal of the order of 10^6 counts.

2.3. *Data processing*

The scattered photon intensity, $I_s(E, P)$, from Li at a pressure P was estimated in the following way, where E is the photon energy. First the X-ray intensity at ambient pressure without the Li sample is observed (*i.e.* the background), $I_0(E)$. It is assumed that the background $I_0(E)$ is independent of pressure. Second, the intensity including the Li sample is observed, $I(E,P)$. It is assumed that $I_s(E,P)$ has the following form,

$$I_s(E,P) = I(E,P) - \alpha(P)I_0(E), \tag{1}$$

where α is an adjustable parameter depending on the pressure. The process to extract the Compton profile $J(q)$ from $I_s(E,P)$ has been described previously (Itoh *et al.*, 1979).

3. Results and discussion

Fig. 3 shows examples of the measured scattered X-ray intensity $I(E,P)$ both at ambient pressure and at 1.8 GPa in the range of channel between 1200 (36.67 keV) and 2000 (60.91 keV). The Compton profile $J(q)$ was obtained by using the observed $I(E,P)$ and the procedure described in §2.3. Examples of $J(q)$ are shown in Fig. 4 for ambient pressure and 1.8 GPa. It is found that the value of $J(0)$ decreases with increasing pressure, which indicates an increase of magnitude in the Fermi momentum q_F at high pressure because of the relation $J(0) \propto q_F^{-1}$ in the framework of the free-electron model (FEM).

Next we show briefly how to get the value of q_F from the observed $J(q)$. In the framework of the FEM, $J(q)$ can be described as

$$J(q) = \frac{3z}{4q_F^3}(q_F^2 - q^2). \tag{2}$$

Here z is the number of valence electrons per atom and q_F is the Fermi momentum given by,

$$q_F = \left(\frac{3\pi^2 N}{V}\right)^{1/3}, \tag{3}$$

where V is the volume and N is the number of electrons.

By differentiating (2) with respect to q, we obtain

$$\rho(q) = -\frac{1}{q}\frac{\partial J(q)}{\partial q} = +\frac{3z}{2q_F^3} = \text{constant}. \tag{4}$$

This result means that $\rho(q)$ is constant in the range, $-q_F \le q \le q_F$. At finite temperature, however, $\rho(q)$ has a finite width of $k_B T$ at q_F *via* the Fermi distribution function. So q_F was determined as the value of q at the full width at half-maximum (FWHM). From this result, we obtained q_F as a function of pressure. q_F is found to increase with pressure having a coefficient, $q_F^{-1}\partial q_F/\partial P = 3.8\times10^{-2}$ GPa^{-1}. On the other hand, using (1), we obtained the change of q_F as $q_F^{-1}\partial q_F/\partial P = (1/3)\kappa$, where κ is the compressibility of Li. By using $\kappa = 0.1$ GPa^{-1} for Li (*e.g.* Olinger & Shaner, 1983), the pressure coefficient is estimated to be 3.3×10^{-2} GPa^{-1}, which is in good agreement with the present result mentioned above.

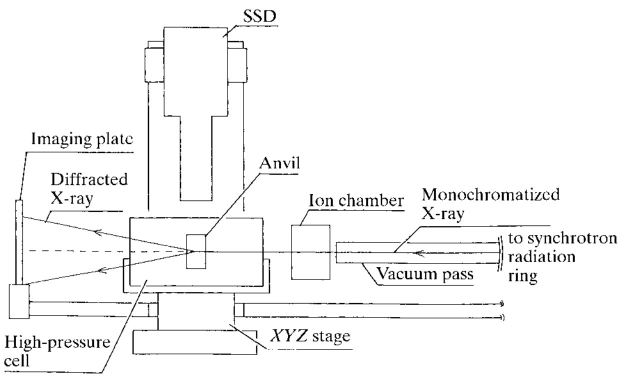

Figure 2
Schematic diagram of the optical system for Compton scattering measurement.

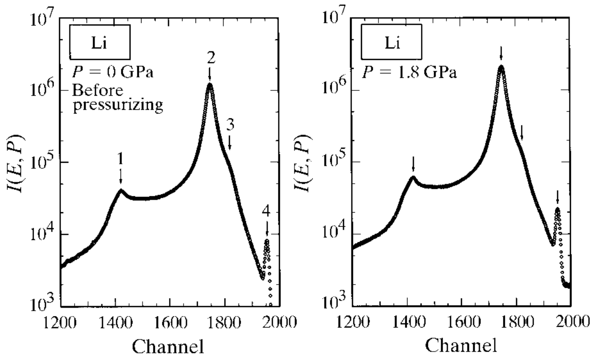

Figure 3
Compton profiles of Li at ambient pressure and 1.8 GPa. The peaks, shown by the arrows, originate as follows: (1) escape peak due to the detector; (2) Compton scattering; (3) background; (4) elastic scattering.

4. Summary

We have constructed a high-pressure apparatus for the measurement of the Compton scattering in metals and alloys using synchrotron radiation. By using this apparatus, we succeeded in observing the increase of the Fermi momentum, q_F, of metallic Li with increasing pressure. The pressure coefficient of q_F was in good agreement with that predicted from the free-electron model. This fact certifies the suitability of the present apparatus and data

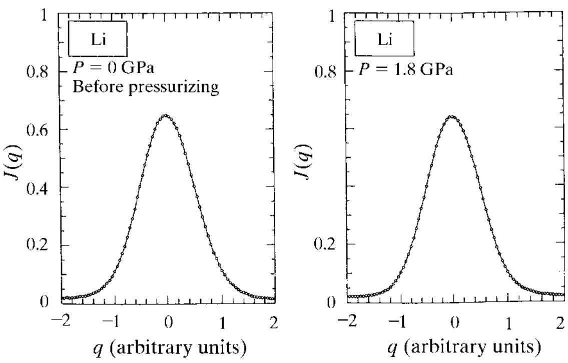

Figure 4
$J(q)$ of Li at 0 GPa (ambient pressure) and 1.8 GPa.

processing to determine the momentum distribution of conduction electrons and the Fermi momentum in metals and alloys.

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