EPR STUDY OF KOREAN NATURAL AMETHYST*

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INTRODUCTION

Electron paramagnetic resonance of natural amethyst mined in Korea has been investigated by employing a Varian X-band spectrometer at room temperature. Complicate lines more than 30 were easily observed with the magnetic field up to 1.05 T on the three mutually perpendicular crystal planes. The signals of S_1 center(1,2) are the most prominent one and exhibit six equivalent sites.

EXPERIMENTAL RESULTS AND ANALYSIS

The observed resonance spectra are analysed in terms of three groups. The most prominent S_1 center is due to substitutional Fe^{3+} at Si^{4+} sites. The second is composed of several lines of five subgroups nearly isotropic on each of the planes at about 525, 337, 272, 125, and 60 mT. The third complex group contains the S_2 center(3) of which EPR parameters are not known yet.

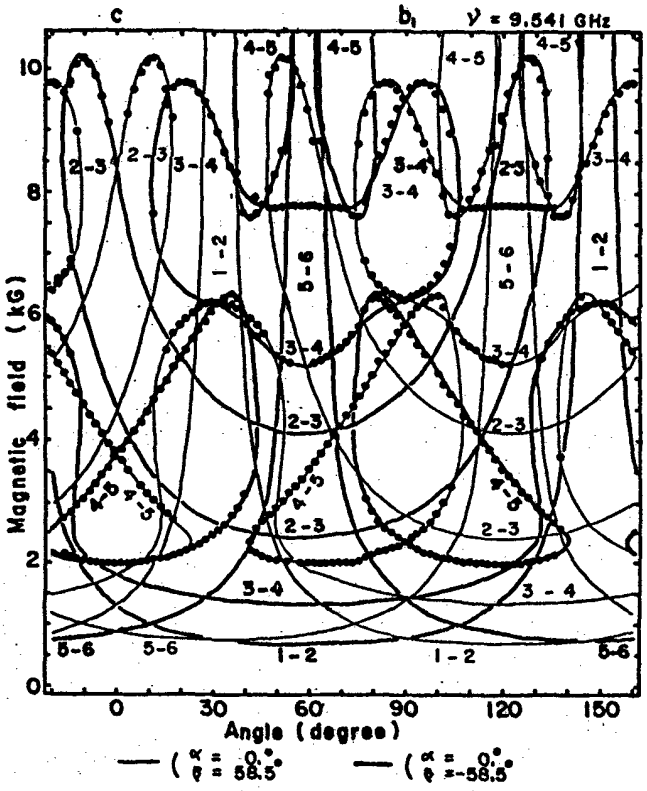

Fig.1 EPR spectra of the S_1 center in the bc-plane.

The spectra of S_1 center are analysed in terms of the orthorhombic spin Hamiltonian with S=5/2, g=2.0032, D= 9.315, E=1.741, and F=-0.0063 GHz. The observed S_1 centers are found to have six equivalent sites having the principal axes as follows: the x-axis of each site taking one of the crystallographic a-axes, the z-axis being $\pm 58.5^{\circ}$ from the c-axis, respectively, rotated about each x-axis, and the y-axis along the direction of $\mp 31.5^{\circ}$ from the c-axis on the bc-plane. Since there are three equivalent Si sites, the S_1 center usually exhibits this symmetry accordingly. However, it is found to have six due to $\pm 58.5^{\circ}$ in natural amethyst.

The calculations of resonance field on the three planes are executed to transform crystallographic axes to each of the principal axes of the Hamiltonian matrix with a rotation matrix of $R_x(\alpha)R_z(\beta)$, where α is 0°, $\pm 120^{\circ}$, respectively, and with β of 58.5° or -58.5°. The resonance fields are well in accord with caculations of six sites on the three crystallographic planes. One of these is shown in Fig.1. Although four among six equivalent sites are distinguished in this plane, the only resonance fields due to two sites with same $\alpha = 0^{\circ}$ are plotted for simplicity. The heavy and light lines are due to the other site with different β. This is a result of two possible handedness of the α-quartz, and confirms the twinning of the crystal. The ratio of intensity of these is about 3:7:19:67:36:4.

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* Supported by the Korea Science and Engineering Foundation (1985-87).