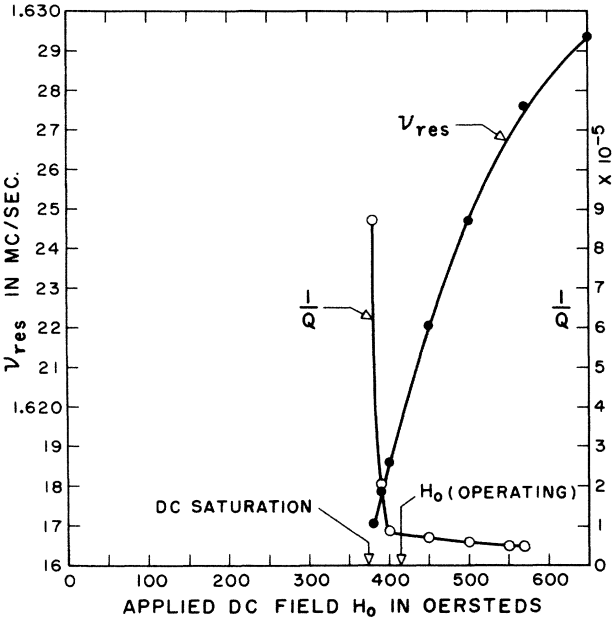

FIG. 1. Plots of ν_{res} and Q^{-1} vs H_0 for a single-crystal EuIG sphere, with H_0 along the [111] axis for the oblate-prolate mode. The H_0 (operating) point was chosen by maximizing the product $Q\nu_{res}^{-1}\partial\nu_{res}/\partial H_0$.

theoretical curve [Eq. (2)]. The minimum threshold h_{crit}(min) was measured as approximately 0.20 Oe. It can be shown for the oblate-prolate mode vibrating with its axis displaced from the z axis (which is the case in our experiments) that the displacement has shear components similar to those in the lowest-order thickness shear mode of a plate. Thus, we expect a comparable though higher threshold for this mode, as shown by the relatively good agreement between the theoretical and observed thresholds.

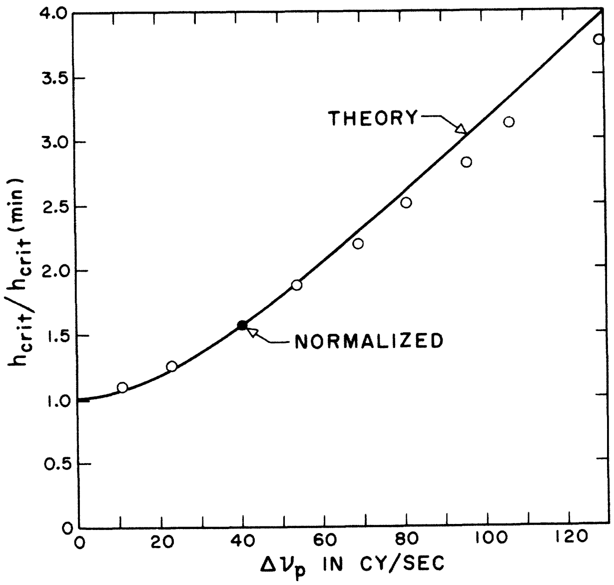

FIG. 2. Comparison of theory and experiment for h_{crit} vs $\Delta\nu_p$.

We expect that this effect can be observed at higher frequencies on either branch of the coupled-mode spectrum, and that also by mechanically loading the elastic mode, acoustic amplification should be possible.

The authors wish to acknowledge discussions with B. A. Auld concerning magnetoelastic instabilities.

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ELECTRON PARAMAGNETIC RESONANCE INVESTIGATION OF THE VACANCY IN DIAMOND

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Griffiths, Owen, and Ward[1] reported that diamonds exposed to reactor neutrons developed an intense isotropic electron paramagnetic resonance (EPR) absorption line whose g value was very close to that of the free electron. They found that a similar line was produced by 1-MeV electrons. The work herein reported has established that this absorption is composed of at least three superimposed lines. Following the precedent established for silicon,[2] they are called the diamond A, B, and C centers. The widths and g values of these lines are listed in Table I. The A- and B-center absorptions are observed with the reference phase of the lock-in detector in

Table I. Full width between absorption-derivative maxima and g values for diamond A, B, and C centers. The magnetic field is in the [100] direction.

Center	ΔH (gauss)	g
A	0.43	2.00230 ± 0.00010
B	1.5	2.00234 ± 0.00010
C	2.4	2.00238 ± 0.00010

phase with the modulation field. On illumination with ultraviolet light, the A-center resonance grows to completely mask that of the B center. The C center is observed with the reference phase in quadrature with the modulation. As will be discussed below, the A center can be shown to be the isolated carbon vacancy.

The stone used in these experiments was a type IIa cleavage which showed a very weak nitrogen[3] EPR signal prior to irradiation. It was irradiated with 0.75-MeV electrons to a total dose of 9×10^{17} electrons/cm^2 at room temperature. This energy favors the production of A centers. The EPR spectrometer used was a standard X-band unit manufactured by Varian Associates. The field modulation frequency was 100 kc/sec. All measurements were performed in absorption at room temperature.

The A-center line shape is Lorentzian except for an unresolved hyperfine interaction with 1.1% abundant C^{13} nuclei. The linewidth is anisotropic, being least in the [111] direction and greatest in the [100] direction. This suggests an unresolved uniaxial g tensor with [100] principal axes. Two sets of resolved hyperfine interactions are observed. The first set is with four equivalent C^{13} nuclei. These are identified as the four vacancy-nearest-neighbor atoms shown in Fig. 1. The second set is with twelve equivalent nuclei. These sites are identified as the twelve second-nearest neighbors. A third set is visible but not resolved. The hyperfine tensors are uniaxial with the four [111] directions as principal axes. The splittings are given in Table II. The resonance is excited by light having an energy greater than 2.83 eV and is quenched by light with an energy greater than 1.10 eV. The quenching curve appears to contain considerable structure. At room temperature the time constant for spontaneous decay is of the order of days.

These results provide experimental confirmation for the theory proposed by Yamaguchi and Kojima,[4] Coulson and Kearsley,[5] and Yamaguchi.[6] The removal of a carbon atom from a lattice site leaves a broken bond protruding from each of the four nearest neighbors as shown in Fig. 1. They assume that the electrons form a defect "molecule," since it is energetically advantageous for these vacancy electrons to delocalize. Coulson and Kearsley call the four protruding orbitals a, b, c, and d. The appropriate one-electron molecular orbitals are

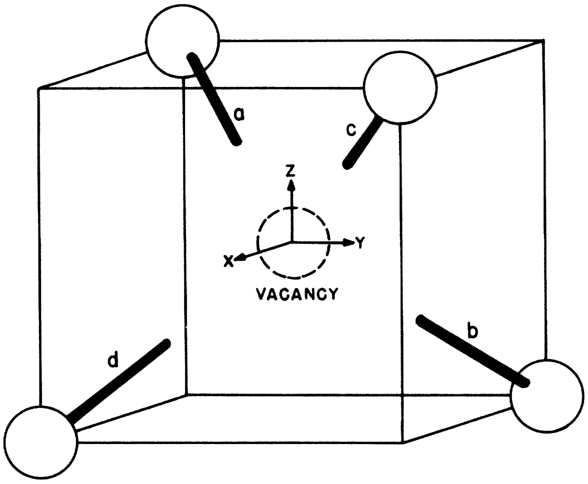

FIG. 1. The four nearest neighbors surrounding a lattice vacancy in diamond. The broken-bond orbitals are labeled a, b, c, and d. The unpaired electron of the positively ionized vacancy is taken to be in an orbital of the form $\Psi = a + b - c - d$.

$$v = a + b + c + d,$$

$$t_x = a + b - c - d,$$

$$t_y = a - b - c + d,$$

$$t_z = a - b + c - d.$$

Table II. Magnetic field separation of hyperfine components due to interaction with the vacancy nearest-neighbor and second-nearest-neighbor C^{13} nuclei. The hyperfine tensors are uniaxial with the four [111] directions as principal axes. The tabulated values are measured parallel and perpendicular to the principal axes.

	$\Delta H_{\parallel}$ (gauss)	$\Delta H_{\perp}$ (gauss)	No. equivalent sites
Nearest neighbor	50.480	29.180	4
2nd-nearest neighbor	4.750	3.320	12

Table III. Values of $|\Psi(0)|^2$ and $\langle r^{-3}(3\cos^2\theta - 1)\rangle$ at vacancy nearest-neighbor and second-nearest-neighbor positions computed from hyperfine data.

	$\lvert\Psi(0)\rvert^2$ (10^{24} cm^{-3})	$\langle r^{-3}(3\cos^2\theta - 1)\rangle$ (10^{24} cm^{-3})
Nearest neighbor	0.61	2.0
2nd-nearest neighbor	0.064	0.13

The calculations indicate that the ground state of the neutral vacancy is a singlet and therefore diamagnetic.

The experimental results may be explained in terms of this model as follows: Light of energy greater than 2.83 eV ionizes neutral vacancies, and the resulting electrons are trapped on some unidentified center (or centers) lying 1.10 eV (or more) below the conduction band. The resulting positively ionized vacancy is assumed to have a v^2 core. The unpaired third electron then occupies one of the three t_2 orbitals. The defect is presumably stabilized by Jahn-Teller distortion. Crude molecular orbital calculations indicate that about 80% of the unpaired electron wave function may be accounted for in this way. This model gives the required quadricentric wave function and predicts, as well, [100] principal axes for the g tensor.

Values of $|\Psi(0)|^2$ and $\langle r^{-3}(3\cos^2\theta - 1)\rangle$ for the unpaired electron wave function at the positions of the nearest-neighbor and second-nearest-neighbor atoms calculated using the relations derived by Abragam and Pryce[7] are given in Table III. Assuming that at the position of the second-nearest neighbor the wave function is essentially sp^3 in nature, the ratio of $|\Psi_{2S}(0)|^2$ to $\langle r^{-3}\rangle_{2p}$ for C in diamond may be calculated. This ratio is found to be 1.14. As would be expected, this is closer to the value 0.955 calculated from hydrogenic orbitals than is the value 1.4 found for silicon.[2] Using this ratio, the degree of hybridization in the broken-bond orbital may be found from the nearest-neighbor hyperfine data. The ratio of s to p character is 0.214, which is less than the perfect crystal value 0.333. This change in hybridization reflects the relaxation of the nearest neighbors away from the vacancy. The change in angle between the broken bond and the orbitals bonding the nearest neighbor to the second-nearest neighbor may be calculated, assuming that the relaxation is radial and that the four atomic orbitals centered on the nearest-neighbor atom must remain orthogonal. This angle is found to decrease from the tetrahedral angle by 3° as a result of the relaxation.

The structure of the diamond vacancy may be compared with that of the silicon vacancy recently reported by Watkins.[8] The two vacancies appear to be qualitatively identical, with the sole exception that the silicon nearest neighbors relax toward, rather than away from, the vacancy.

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