

COMMENT

Comment on ‘Evidence for a Fe-related defect centre in diamond’

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Abstract

Recently, we have characterized the 1.789 eV photoluminescence (PL) centre in diamond grown by a high-pressure high-temperature technique (Yakubovskii K and Adriaenssens G J 2002 *J. Phys.: Condens. Matter* **14** L95). In this communication, we demonstrate that this PL centre most probably originates not from a point defect in diamond, but from crystalline $\text{Al}_2\text{O}_3:\text{Cr}^{3+}$ (ruby) inclusions in diamond.

The following properties of the 1.789 eV centre have been reported in our previous work [1]:

- (1) At room temperature, the centre consists of two narrow (width ~ 1 meV) zero-phonon lines (ZPLs) at 1.7869(3) and 1.7906 eV accompanied by two weak vibronic peaks, red-shifted by 30 and 48 meV from the ZPLs. The lifetime of the ZPL intensity is ~ 7 ns.
- (2) Cooling the 1.789 eV centre from 300 to 77 K induces the following changes: the positions of both ZPLs shift by +2.4 meV without significant change in their relative intensity; the ZPL width decreases by $\sim 50\%$ and the lifetime increases by $\sim 50\%$.
- (3) The excitation spectrum of the centre, measured in the range 2.0–2.7 eV at 300 K, shows a broad band (width ~ 0.2 eV) peaking at 2.25 eV.
- (4) The centre is observed only in nitrogen-free high-pressure high-temperature (HPHT) crystals grown in an Fe-containing chamber. In those samples, the centre is spatially concentrated around Fe-containing inclusions.

On the basis of the above observations it was concluded that the ZPL doublet originates from optically forbidden transitions between an excited state and a ground state split by 3.6 meV at a defect centre in diamond. The defect was thought to involve an interstitial Fe atom.

Recently, we have recognized that measurements in the temperature range 77–300 K could not conclusively decide whether the 3.6 meV splitting occurs in the ground or in the excited state of the 1.789 eV centre. Therefore, additional PL measurements have been performed at lower temperatures (down to 10 K), on a larger series of samples. The newly obtained results are briefly summarized below:

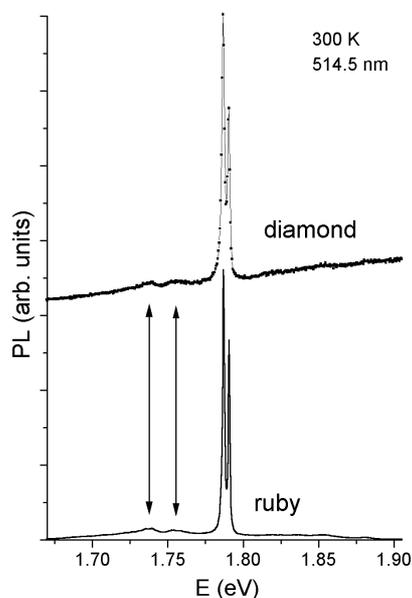


Figure 1. PL spectra recorded at 300 K under 514.5 nm Ar⁺ laser excitation from an HPHT diamond and ruby sample.

- (5) The ratio of the high-energy to low-energy ZPL intensity decreases with cooling at $T < 30$ K, revealing that the 3.6 meV splitting occurs in the excited state, but not in the ground state as reported previously. No significant change in the ZPL position, width and lifetime was observed in the temperature range 10–80 K.
- (6) The centre was also detected in small (~ 0.5 mm) HPHT diamond crystals with relatively high average nitrogen concentration (~ 200 ppm). Interestingly, although those samples were grown in a ‘pure’ Mg–Cu–C medium, IR absorption and PL measurements, assisted with an optical microscope, revealed the presence of boron and Ni impurities in different growth sectors of those crystals.
- (7) Photoluminescence excitation (PLE) measurements were extended to 3 eV. An extra signal at ~ 2.7 eV, exhibiting the same intensity and width as the 2.25 eV band, has been detected.

We have further noticed a remarkable similarity between the optical parameters of the 1.789 eV centre in diamond and Cr³⁺ in crystalline Al₂O₃ (ruby). In order to make an accurate comparison, Raman, PL and PLE measurements were performed under the same conditions on an HPHT diamond crystal and a laser-quality ruby sample (Cr³⁺ content 0.05%). Within our experimental accuracy, we observe no differences in the line position (see figure 1), width, lifetime and their temperature dependencies, or in PLE spectra for the 1.789 eV centre in diamond and Cr³⁺ in Al₂O₃.

Therefore, we conclude that the 1.789 eV PL centre in diamond probably originates from inclusions of ruby trapped from the material of the HPHT chamber during the diamond growth. Those inclusions could not be detected by means of Raman scattering or optical microscopy in our samples, thus suggesting the inclusion size to be no larger than a few micrometres.

References

- [1] Iakoubovskii K and Adriaenssens G J 2002 *J. Phys.: Condens. Matter* **14** L95