Chapter 15
Conclusions and Outlook

15.1 Conclusions

One basic idea for this book was to split up the huge number of spectral lines into 27 tables (see Chaps. 2–7), based on the two criteria, (a) the type of sample and (b) the method of observation. A further aim was the interpretation, i.e., assignment of the lines to specific defects, and (hopefully) identification of the corresponding structure.

Structure assignments: This handbook is a breakthrough in the understanding of the large number of spectral lines in diamond. Data on more than 2,000 lines and bands are presented in 200 tables, including many unpublished results.

With a novel organization scheme, the search for a specific line is greatly simplified as a benefit for researchers and students.

In order to meet the interest in the understanding of the spectra, structure assignments for 80% of the lines are given, of which 15% only were published before. The majority of the structures for the 300 centers is explained in most cases for the first time.

Examples for successful structure assignments are: The infrared centers D = platelets =* $(C_{2n})_i^\circ$, E =* N_1^+, F =* $V_1N_4(C_2)_i^\circ$, and the visible or ultraviolet centers TR12-TR17 =* $(C_2)_i^-$, and N9 = $V_1N_4^-$.

Donor–acceptor pair (DAP) transitions: A considerable progress is achieved by the identification of 97 donor–acceptor pairs (116 DAP entries in Table 10.1), which (with two exceptions: DAP1 [Dis94a, Dis94b] and DAP2 [Ste99a, Ste99b]) are published for the first time. The group of lines GR2–GR8, which for many years was a "basic puzzle," is now explained by DAP32. The DAP results are of great help when discussing the defect structures.

Sideband type DAPs: These occur exclusively with intrinsic defects (vacancies, interstitials, and their associates). If a sideband DAP is found, the respective center must contain an intrinsic defect. Conversely, if the ZPL of a center with an intrinsic

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defect is found, one can look for DAP transitions, which can be weak enough to be overlooked (see Table 10.1).

Depth of donor centers: In Table 10.3, the depth of five deep nitrogen centers (E_D between 1.44 and 3.48 eV) are listed, together with 2.59 eV for oxygen and 0.62 eV for the shallow phosphorous donor.

Dependence of the dielectric factor D on the total number of electrons: For neutral DAP centers, there is a close relationship between the dielectric factor *D* and the total number of electrons. This allows to determine the number of ligand carbon atoms involved (see Table 10.4).

Dependence of the dielectric factor D on the charge state: In Table 10.5 an empirical law is demonstrated. Going from the negative charge state over neutral to the positive charge state, the dielectric factor is increased by 0.05–0.16 eV with an average of 0.11 eV. One surprise was the positive charge state of the GR2-8 center (V_1^+). This explains the intense photoconductive response of GR2-8.

Transition metals: Until recently, only six nickel centers were described [Col97b]. In Tables 9.5.1.1–9.5.1.2 the present knowledge on 20 nickel centers with eight standard DAPs (S2-*S9), and eight sideband DAPs, and four centers without DAP lines are listed.

Surprisingly, cobalt centers in diamond were unknown until a pioneering article appeared [Law96]. In Table 9.6 all observed lines are assigned to six cobalt centers, including three sets of DAP transitions.

Of the other solvent metals, only lines from chromium and iron are found (see Table 9.7.2). Using doping or ion implantation, optical centers of Ti, Zn, Zr, Ag, Ta, and W have been produced (see Table 9.7.2).

15.2 Outlook

Continued research is necessary for a better understanding of those optical centers in diamond, which have only a proposed assignment and structure (marked by a preceding *). Also, there are still 20% of the lines, which are not yet assigned.

Spectra: A better signal-to-noise ratio is desirable for many DAP transitions. Often, these sidelines are weak and were of no interest before the present DAP analysis.

Isotopes: One powerful method in defect structure assignment is isotopic line shift analysis: (^{2}H, ^{13}C, ^{15}N, ^{29}Si, ^{30}Si, ^{60}Ni, ^{62}Ni, see Tables 7.1–7.5). Especially,

partial isotope substitution can reveal the number of atoms involved (e.g., 3 lines for $^{*}(N_2)_i^{\circ}$ (see Table 7.3) or 5 lines for $^{*}(V_4D_4)^{\circ}$ (see Table 7.1).

Photoconductivity spectra: In Chap. 10 of [Zai01], 59 PC peaks or thresholds are listed. Until now, only in few cases a correlation with optical centers is given. The defects with DAP transitions are good candidates for PC measurements. Two excellent examples, where optical absorption and PC spectra coincide, are $^{*}V_1^{+}$ – DAP32 = GR2-8, and $^{*}V_1N_4^{-}$ – DAP63 = N9(a).

Electron spin resonance: More ESR results are desirable. Many defects have several charge states (see Table 10.5) and are probable candidates for ESR measurements.

Correlations: It is important to measure for one particular sample the optical lines in different spectral regions. Until the pioneering work with IR and UV correlation appeared [Naz87], the well known A, B, and C centers were regarded as isolated IR centers, ignoring their UV lines. It is expected, that, more such correlations can be established. An elegant proof for the correlation of two charge states of the same defect is the quantitative photochromic interconversion between two spectra (e.g., V_1° = GR1 and V_1^{-} = R10 = ND1). Many more defects exist in several charge states (see Table 10.5).

Theory: The theoretical treatment of defects in diamond should be extended. Theorists can hopefully provide a comprehensive treatment for the new field of DAP transitions, including the phenomenon of high intensity shells, and the near shell correction.

Nanodiamond: These new materials (nanowires, nanoparticles) are of high interest for applications. A comprehensive description of the *optical* properties is desirable.