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# A web-based database for EPR centers in semiconductors

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**Abstract**

We develop a web-based database system for electron paramagnetic resonance (EPR) centers in semiconductors. This database is available to anyone at http://www.kc.tsukuba.ac.jp/div-media/epr/. It currently has more than 300 records of the spin-Hamiltonian parameters for major known EPR centers. One can upload own new records to the database or can use simulation tools powered by EPR–NMR©. Here, we describe the features and objectives of this database, and mention some future plans.


*Keywords:* EPR; Database; Semiconductor; Defect

## 1. Introduction

Electron paramagnetic resonance (EPR) or electron spin resonance (ESR) spectroscopy is widely used to study defects and impurities in semiconductors. Its first application to semiconductors was reported in 1953 for Si [1]. Since then, more than 410 EPR centers in Si have been reported [2]. In addition, Ge, diamond, GaAs, and recently GaN, SiC, ZnO, and other new semiconductors have been studied using EPR, resulting in a large accumulation of EPR data so far. EPR spectroscopy provides unique information about the wave function of a paramagnetic center, which can be directly compared with the results of first-principles calculations, leading to a number of confident identifications of defects and impurities. With this valuable feature, it will be continually applied to semiconductors in the future.

However, a troublesome problem with EPR for semiconductors is that, unlike in other spectrographic techniques, the spectroscopic data can not be simply described based on where resonant peaks are observed with the scanning of the excitation energy. This is because the EPR spectrum is drastically changed by a crystal orientation with respect to the applied magnetic field. Furthermore, there are many duplicate peaks in the spectrum due to the presence of symmetry-related sites in a crystal. Traditionally, EPR data have been described in terms of a set of the spin-Hamiltonian (SH) parameter tensors, from which we can simulate a set of peak positions for a certain experimental condition. Of course, this simulation process requires special software as well as a deep understanding of the SH calculation.

Due to these problems, even EPR specialists often find it difficult to accurately compare EPR spectra. This has become a barrier to EPR studies, and the barrier is getting higher as the number of reports increases. Thus, to minimize this barrier and establish a more efficient and convenient system for accumulating EPR data, we have developed a web (world wide web)-based database, named EPR in Semiconductors [3]. This database is now accessible to anyone from anywhere via the Internet.

## 2. Two foresightful works

Before we introduce EPR in Semiconductors, we must mention two foresightful projects that guided us in designing the database.

One is the big web-based database for EPR named the Spin Trap DataBase (STDB) [4]. The STDB contains more than 10,000 records of spin traps that are used extensively in chemical, medical, and biological science. To collect such a large number of records, many contributors are absolutely necessary. For this purpose, it is important to

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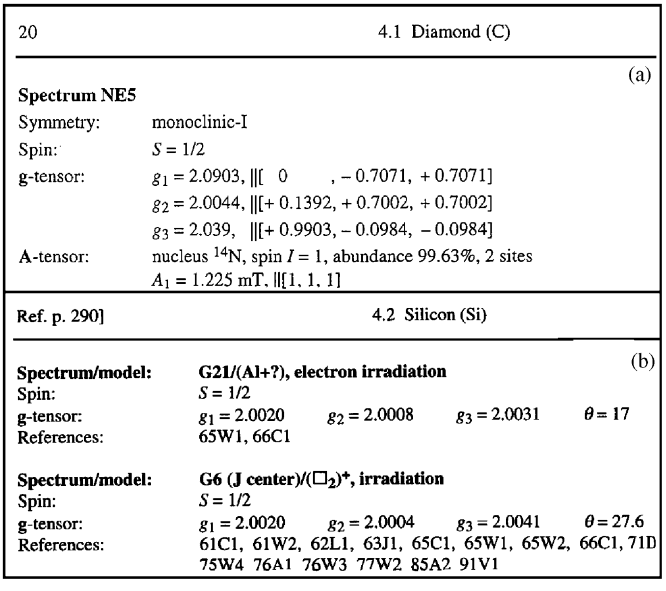
design a simple and flexible electronic format for EPR data, one that can be handled easily by any experimentalist. In STDB, this issue is less important because of the isotropic nature of spin traps in liquid. Defining a spin trap only requires a set of the g and hyperfine (HF) *constants*. For semiconductors, however, one must define not only a set of SH *tensors* but also *symmetry-related sites* of the relevant crystal.

The other is the new Landort–Börnstein series which makes a great effort to accumulate all the reported SH parameters for semiconductors (Fig. 1). We believe that this is the most sophisticated and knowledgeable compilation of EPR centers in semiconductors. However, the ways the SH tensors are described are not unique even in this excellent reference. For example, as shown in Fig. 1(a), the tensors for diamond are expressed by principal values and principal axes [5], while for Si [Fig. 1(b)] the principal values and a characteristic angle ($\theta$) are given instead [2]. Furthermore, these axes or angles have to be changed when we choose a different coordinate for a spin system. This complication also appears in official journals, where the SH parameters are expressed in a variety of formats or coordinates. We should also point out that, even using the well-defined data like in Fig. 1, there remains the complicated problem of calculating a set of peak positions, as we mentioned already.

Accordingly, the best way to accumulate EPR data is to electronically store the SH parameters in a web-based database like the STDB. We could use them to simulate a set of peak positions for any experimental conditions we desire. For this purpose, we need (1) an appropriate electronic format for EPR data, (2) an appropriate simulator that can handle the above format, and (3) an appropriate web-based interface to offer the services of the database.



20 4.1 Diamond (C)

(a)

**Spectrum NE5**

| | |
|---|---|
| Symmetry: | monoclinic-I |
| Spin: | $S = 1/2$ |
| g-tensor: | $g_1 = 2.0903$, \|\|[ 0 , − 0.7071, + 0.7071] |
| | $g_2 = 2.0044$, \|\|[+ 0.1392, + 0.7002, + 0.7002] |
| | $g_3 = 2.039$, \|\|[+ 0.9903, − 0.0984, − 0.0984] |
| A-tensor: | nucleus $^{14}$N, spin $I = 1$, abundance 99.63%, 2 sites |
| | $A_1 = 1.225$ mT, \|\|[1, 1, 1] |

Ref. p. 290] 4.2 Silicon (Si)

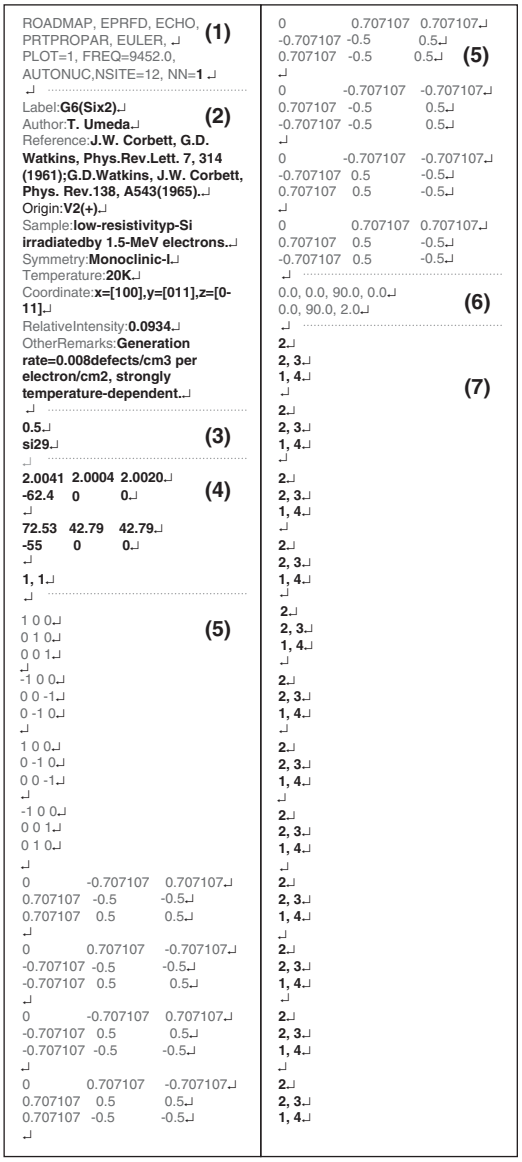
(b)

| | | | | |
|---|---|---|---|---|
| **Spectrum/model:** | **G21/(Al+?), electron irradiation** | | | |
| Spin: | $S = 1/2$ | | | |
| g-tensor: | $g_1 = 2.0020$ | $g_2 = 2.0008$ | $g_3 = 2.0031$ | $\theta = 17$ |
| References: | 65W1, 66C1 | | | |
| **Spectrum/model:** | **G6 (J center)/($\square_2$)*, irradiation** | | | |
| Spin: | $S = 1/2$ | | | |
| g-tensor: | $g_1 = 2.0020$ | $g_2 = 2.0004$ | $g_3 = 2.0041$ | $\theta = 27.6$ |
| References: | 61C1, 61W2, 62L1, 63J1, 65C1, 65W1, 65W2, 66C1, 71D 75W4, 76A1, 76W3, 77W2, 85A2, 91V1 | | | |

Fig. 1. The new Landort–Börnstein series for EPR centers in (a) diamond and (b) Si, after Refs. [5] and [2], respectively. Note that both pages summarize EPR centers of monoclinic-I symmetry, while their expressions are apparently different.

## 3. The web-based database: EPR in Semiconductors

To satisfy the above requirements, we adopted the simulation program EPR–NMR©, which was developed by the group of Profs. Weil (University of Saskatchewan, Canada) and Mombourquette (Queen's University, Canada) [6]. One of us (J. Isoya) contributed to the development



```
ROADMAP, EPRFD, ECHO,                                   (1)
PRTPROPAR, EULER,
PLOT=1, FREQ=9452.0,
AUTONUC,NSITE=12, NN=1
Label:G6(Six2)                                          (2)
Author:T. Umeda
Reference:J.W. Corbett, G.D. Watkins, Phys.Rev.Lett. 7, 314 (1961);G.D.Watkins, J.W. Corbett, Phys. Rev.138, A543(1965).
Origin:V2(+)
Sample:low-resistivityp-Si irradiatedby 1.5-MeV electrons.
Symmetry:Monoclinic-I
Temperature:20K
Coordinate:x=[100],y=[011],z=[0-11]
RelativeIntensity:0.0934
OtherRemarks:Generation rate=0.008defects/cm3 per electron/cm2, strongly temperature-dependent.
0.5                                                     (3)
si29
2.0041  2.0004  2.0020                                   (4)
-62.4   0       0
72.53   42.79   42.79
-55     0       0
1, 1
1 0 0
0 1 0                                                   (5)
0 0 1
-1 0 0
0 0 -1
0 -1 0
1 0 0
0 -1 0
0 0 -1
-1 0 0
0 0 1
0 1 0
0          -0.707107   0.707107
0.707107   -0.5        -0.5
0.707107   0.5         0.5
0          0.707107    -0.707107
-0.707107  -0.5        -0.5
-0.707107  0.5         0.5
0          -0.707107   0.707107
-0.707107  0.5         0.5
-0.707107  -0.5        -0.5
0          0.707107    -0.707107
0.707107   0.5         0.5
0.707107   -0.5        -0.5
0          0.707107    0.707107
-0.707107  -0.5        0.5
0.707107   -0.5        0.5                              (5)
0          -0.707107   -0.707107
0.707107   -0.5        0.5
-0.707107  -0.5        0.5
0          -0.707107   -0.707107
-0.707107  0.5         -0.5
0.707107   0.5         -0.5
0          0.707107    0.707107
0.707107   0.5         -0.5
-0.707107  0.5         -0.5
0.0, 0.0, 90.0, 0.0                                     (6)
0.0, 90.0, 2.0
2
2, 3
1, 4                                                    (7)
2
2, 3
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```

Fig. 2. Record file format for the EPR in Semiconductors database. This example defines the famous G6 center (+1 divacancy) in Si. In general, only highlighted parts have to be changed to prepare a record file. There are seven sections: (1) commands to execute the EPR–NMR© simulator, (2) comment lines to supply helpful information regarding this record, (3) electron spins ($S$) and nuclear spins ($I$) (for this case $S = \frac{1}{2}$ and $I = \frac{1}{2}$ of $^{29}$Si), (4) SH parameter tensors (here, a g tensor and a $^{29}$Si HF tensor), (5) 12 rotation matrices for a diamond-type crystal, (6) angular parameters to specify a crystal rotation, and (7) a transition table. Further details can be found in Ref. [3].

of this program. We believe that it is one of the most powerful simulation tools for EPR specialists, and it is certainly one of the most popular. Using the format of this program, many experimentalists will be able to prepare new record files by themselves. With the official permission of Prof. Weil and Prof. Mombourquette, we have joined EPR–NMR© to our web service program.

The record format for the database is shown in Fig. 2. This format is basically the same as used for a "ROAD-MAP" simulation of EPR–NMR©, which calculates an angular map of the resonant fields with respect to a crystal's rotation. In principle, one record is defined by one text file. The file consists of Sections (1)–(7). In Section (4), two SH tensors are defined by a set of three principal values and three Euler angles. A simple matrix expression is also available. Although the expressions of these tensors are changed by the choice of coordinate, consistent simulated results can always be obtained regardless of the expressions or coordinate. To create a new record as easily as possible, please reuse a similar record in the database and modify the highlighted parts only. It is also quite possible to define very complicated spin systems, such as high-spin systems, multi-nuclei systems, and spin systems involving higher-order SH terms. More details about how to prepare new record files can be found in our web pages (see the Help pages) or in the original EPR–NMR© manual.

The database system is composed mainly of the components shown in Figs. 3(a)–(e). Their functions and instructions are as follows.

(a) *Outputs*: Users can obtain their desired outputs by simply clicking on the Spin-Hamiltonian Parameter List [Fig. 3(b)]. One can download original record files or one can simulate angular map or EPR spectrum or energy level, as shown in Fig. 3(a). Three types of simulations can be executed for any experimental conditions, making it possible to directly compare your experimental data with the recorded ones. Or using the original files, one can

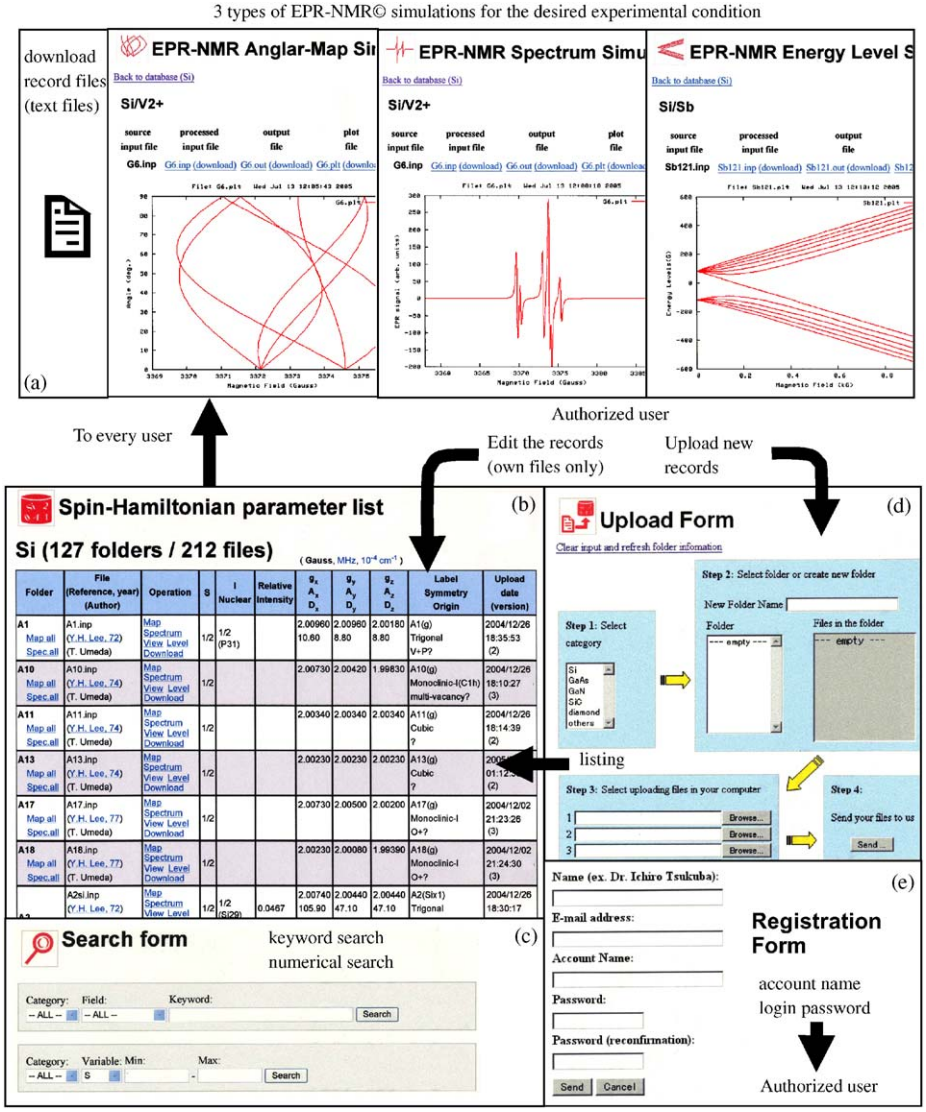


Fig. 3. The whole EPR in Semiconductors system [3].

execute higher-grade simulations on own computer. When a user executes a simulation, three text files will be returned to the user. One file (.out) contains the principal values and axes of each SH tensor in terms of various expressions, which greatly helps in understanding. The print file (.plt) contains plot data for creating original graphs.

(b) *Spin-Hamiltonian Parameter List*: This is the main interface of the database, and allows anyone to easily select records and obtain various outputs as shown in Fig. 3(a). The database is classified into six categories: Si, GaAs, GaN, SiC, Diamond, and Others. Using this interface, authorized users, who have registered the Registration Form [Fig. 3(e)], can edit or delete their own record files. For each record, the updated version is automatically given, as shown in the Figure. To ensure the reliability and security of the database, no one can modify record files that have been uploaded by others. Therefore, if a center is still controversial, there may exist two or more folders/files that have been uploaded by different groups for the center. Users themselves judge which is the better one.

(c) *Search Form*: Both numerical search and keyword search are available. Using this form, the desired EPR data can quickly be found in the database.

(d) *Upload Form*: New records (text files) can be uploaded to the database from here. Firstly our server checks whether the uploaded files have a valid EPR–NMR© format. If the check is okay, then an author who uploaded the files will receive angular-map simulation results (see Fig. 3(a)) so that the author can confirm visually whether those files have been correctly prepared. Finally, the records are listed in the Spin-Hamiltonian Parameter List [Fig. 3(b)].

(e) *Registration Form*: This authorizes a user to upload new files to the database. Simply enter account name and password, together with personal information (name and e-mail address), and our server automatically registers the user. The personal information is used only for non-commercial communication from us to the registered person.

At present, the database contains about 300 records of the major known defects reported from the 1960s to the 1980s. For more recent EPR results, we plan to directly ask researchers to upload their works to the database. Hopefully, this database will contribute to an efficient accumulation, maintenance, and reuse of knowledge about EPR centers in semiconductors. We can of course help the preparation of record files when someone contacts us (see the contact page [3]).

Lastly, we should clarify the important relationship between the journals and this database. The database does not include a screening system. Therefore, the publication of EPR data in an official journal is absolutely necessary for their complete authorization. When one publishes any SH parameters recorded in the database, please cite the original references. If one publishes any outputs (e.g., simulated results) generated by the database system, please cite this database.

## 4. Conclusion

We have developed a web-based database for EPR centers in semiconductors. The database offers very useful simulation services powered by EPR–NMR©, which makes it quite easy to compare one's EPR data with the others. Please try the database and please upload new data. In doing so, an up-to-date and continuously expanding database of EPR centers will be formed, which expectedly contributes to further progress in the EPR research of defects in semiconductors.

## Acknowledgements

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