A Database for Solid State Laser, Optical, and Nonlinear Materials

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ABSTRACT

Solid-state laser models require data for laser, optical, and nonlinear materials. Depending on the particular concern being addressed by a specific model, a broad range of parameters, including, but not limited to, crystalline, optical, thermal, and mechanical properties may be required. Many materials have been investigated as potential laser or nonlinear materials: new materials continue to be developed. Topical concerns, such as atom-to-atom energy transfer and up-conversion, force laser researchers to reassess old data in a new light. The breadth of the data requirements, the large number of materials, the necessity for future expansion, and the changing analytical requirements necessitate a versatile and flexible approach to data storage and retrieval. A computerized, interactive data base which retrieves material data in a way that is useful to the laser designer solves the problem. Such a data base, one part of a larger software package for designing new lasers and assessing the performance of existing lasers, is being developed in the Flight Electronics Division at the NASA Langley Research Center.

1. INTRODUCTION

Active sensors from ground-based and airborne platforms have been used over the past 20 years to investigate atmospheric chemistry and dynamics.[1,2] Passive remote sensors measure either the solar energy transmitted by or reflected from the atmosphere or the energy emitted by the atmosphere itself. Using the received radiation, the total burden of various atmospheric constituents can be determined. Active sensors incorporate their own light source and measure energy backscattered from the atmosphere. The active sensors's light source is generally a pulsed laser beam. Using active sensors, the concentration of various atmospheric constituents can be determined as a function of range. Concentration as a function of range is mandatory if the dynamics and chemistry are to be determined.

Efforts are under way at the NASA Langley Research Center (NASA-LaRC) to develop active sensors to perform Earth sciences experiments from spaceborne platforms. As part of the active sensor development program, NASA is developing solid-state lasers which lase throughout the .280 to 10.0 μm band.[3]

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The unique demands of space-based lasers used for atmospheric remote sensing necessitate development of a laser, nonlinear, and optical materials' database and of solid-state laser models for designing lasers. In general, spaceborne instruments are required to have high reliability, long life, low weight, small volume, relative temperature insensitivity, and low electrical power consumption. Since active atmospheric remote sensors monitor only one atmospheric absorption line, the lasers are required to have a narrow spectral bandwidth, low-amplified spontaneous emission, high output light power, and a moderate pulse-repetition frequency. The low electrical spacecraft power requirement, together with the high output light power requirement, generates a requirement for high electrical-to-optical laser efficiency. Nonlinear optics may be required to convert the laser output to a different wavelength. The combination of constraints on the solution, a large search field, and complex mathematical models makesnecessary the development of laser models which are tied closely to a materials' database. Furthermore, since many laser engineers are not computer experts, the software system should be very user-friendly. Such a database and laser modelling software system is being developed in the Flight Electronics Division, Langley Research Center.

2.0 OVERVIEW

The laser modelling software can be divided into three parts: database LASERS, the laser models, and the interface software. Database LASERS contains the physical properties of laser, nonlinear, and optical materials which are used by the laser models. The laser models can be divided into four classes: efficiency calculations, two electro-optical component models, laser amplifier, resonator, oscillator models, and miscellaneous models. The interface software provides an interactive, user-friendly interface between the user and his personal data files, the laser models and database LASERS. The software currently resides on an IBM PS/2 model 80 computer equipped with a math co-processor chip, 4 MByte of RAM, and a 70 MByte hard disc. The operating system is DOS 3.3.

Database LASERS is subdivided into two parts, spectra and tabulated data. The spectra are ASCII files of laser material's absorption spectra, laser material's emission spectra, and laser diode emission spectra. The tabulated data contains physical properties of laser, optical, and nonlinear materials which runs under the commercially available database manager, R:BASE for DOS. Crystalline, optical, thermal, and mechanical properties, among others, are located in about 25 tables with approximately 190 unique columns of data. Macros, programs written in Standard Query Language (SQL), the database language, retrieve information for the user.

Table 1 summarizes the laser models completed to date. Several models are tied very closely to the database. In particular, the absorption efficiency models[4,5] and radial distribution of absorbed energy model require absorption spectra. The sensitizer transfer rate using Dexter integrals[6] model requires both an active atom absorption spectrum and a sensitizer emission spectrum. A sensitizer transfer rate calculated from energy levels model is currently under development and, as its name implies, requires tabulated data. Most models require the index of refraction and thermal expansion coefficients. As can be inferred, the database is an integral component of the software system.

The menu-driven interface software enables a user to use the laser models and the database without requiring the user to know the directory structure, program names, or macro names. Using the interface software, a user executes the software from his personal directory. Each user's directory stores his personal data files. An individual's file may contain input parameters for a specific model or the results of a model's calculations. At run-time, materials data is available from the database and software is available from the software library.

3.0 SPECTRA

3.1 Absorption Spectra

Transmission and absorption spectra are acquired on a Perkin-Elmer IR-9 spectrophotometer. For isotropic materials, unpolarized spectra are recorded. For uniaxial and biaxial materials, such as Nd:YLF and Nd:YVO_4, polarized spectra are recorded. The spectra are transferred from the PerkinElmer's host computer, a Perkin-Elmer 3600 Data Station, to an IBM PC where headers are added to the files to identify the contents of the spectra. Absorption spectra are converted to transmission spectra. Data processing is used to correct transmission spectrum for Fresnel losses and, if required, for baseline drift. To correct the transmission spectrum for Fresnel losses, the transmission spectrum at each wavelength is multiplied by $(n+1)^4/16n^2$ where n is the index of refraction. The index of refraction must be calculated at each wavelength to preserve accuracy. Although the refractive indices are known, Sellmeier coefficients are not always available from the literature. When the Sellmeier coefficients are not available, refractive index data are fitted to a standard Sellmeier equation of the form

$$n^2 = A + B\lambda^2/(\lambda^2 - C) + D\lambda^2/(\lambda^2 - E)$$

where n is the index of refraction, and λ is the wavelength. After correcting the spectrum for Fresnel losses, the spectrum is corrected, if required, for measurement artifacts. The units are standardized to the absorption coefficient for unity concentration as a function of wavelength from the corrected transmission using

$$\beta_1 = - \ln(T)/(N_c * l)$$

where T is the corrected transmission, Nc is the active atom concentration in the sample, and l is the sample length. The active atom concentration, which ranges from 0 to 1.0, is defined as the fractional substitution of the dopant into a particular site. Finally, a summary of the spectrum's header is stored in the tabulated section of the database and the spectrum is added to the database. A macro allows the user to easily determine the file name of a desired spectrum.

3.2 Emission Spectra

The emission spectra are acquired on a SPEX model DM1B monochromator. Although emission spectra data processing is similar to the absorption spectra data processing, there are some differences between the processing techniques. The emission spectra are not corrected for Fresnel losses although they can be corrected for baseline drift. Further, the emission spectra are scaled to set the peak intensity to one.

Laser diode emission spectra are measured and stored in the database[7]. The spectral distribution of the diode laser pump array is measured using a 0.75 meter Czerny-Turner spectrophotometer with a resolution of 0.02 nanometers. The heat-sink temperature of the array is actively controlled during the measurement. The pulse-repetition rate can be varied from 10 to 50 Hertz and its width can be varied between 10 and 400 microseconds. The relative intensity versus wavelength data is recorded using Boxcar averaging. A computer interface digitizes the information and stores the data on a binary file. Binary files are converted to ASC II files, identifying headers are added to the files, and the spectra are stored in the database.

3.3 Spectra Headers

File headers allow a user to identify the contents of a data file. Table 2 shows the first few lines of a spectra from the database. The header indicates that the spectra contains the absorption for unity concentration for a room temperature 1.80 mm long YAG crystal doped with .0010 atomic Tm. The spectra was taken between .5000 and .8300 micrometers with a resolution of .0001 micrometers. Since YAG is isotropic, both the source and sample were unpolarized. The spectra was taken by someone with the initials MS. MS added the header on January 28, 1988, at 2:56 p.m. The header is terminated by the EOH (End-Of-Header) record. Comments indicate the source of the sample and observations concerning the sample. The header and the data sections are delimited by an End-Of-Header record. The EOH record indicates to the software that the format and contents of the file are about to change: the format changes from alpha-numeric values to numeric values; and the file content changes from the header information to the data section. The record immediately following the EOH record contains the number of data points in the data section of the file. Finally, the spectrum itself is given. In our example, only the first few lines of the spectrum are listed. Absorption spectra contain only one column of data, the absorption for unity concentration. When accessing the data, the wavelength for each data record is calculated from the minimum wavelength and resolution given in the header. As can be seen, headers allow users to identify the contents of a file long after the file has been created. Headers also allow users who did not create a file to easily determine the contents of the file. Most files associated with the laser modelling system contain file headers.

4.0 TABULATED DATA

4.1 Contents of the Tabulated Database

The tabulated section of Database LASERS can be divided into several parts: crystalline, optical, mechanical, thermal, and miscellaneous data. Since each entry in the database is footnoted, the source of each piece of data can be easily determined. Macros, user-friendly, interactive programs written in the R:BASE Standard Query Language (SQL) language, have been created to load, retrieve, and maintain database LASERS. Macros for retrieving data from the database will be discussed below. Macros for loading data into the database and maintaining the database (e.g. backing up the tables) will not be discussed here.

Absorption - emission filenames contain spectra filenames plus approximately 25 parameters taken from the file headers. The parameters, such as laser material, active atom, source and sample polarization, minimum and maximum

wavelength, and resolution, enable a user to identify the spectra. This table and its associated macros enable a user to easily determine which spectrum is required for his particular needs.

Chemical names and formulas contain common names and chemical formulas for commonly used materials. Since most data in the database is cataloged by chemical formula, this table allows the user to easily switch from the solid-state laser jargon to the scientific name. For example, YAG could be identified as $Y_3Al_5O_{12}$. The latter name would be the name under which the information would be found in other database tables.

Laser crystal properties include energy level energy, degeneracy, identification, line width, line strength, peak cross-section, and branching ratio for each energy level in the manifold and lifetime for each manifold. Laser crystal properties vary as functions of active atom, laser material and temperature.

Mechanical properties include damage threshold, density, Poisons' ratio, yield strength, and Young's modulus for laser, optical, and nonlinear materials. Some mechanical properties depend on the crystal axis as well as the material. As such, some quantities become tensor quantities.

Optical properties include the Sellmeier coefficients and the change in index of refraction with temperature. Nonlinear coefficients are also included for nonlinear materials. Optical properties vary with optical axis. When available, the temperature dependence of these parameters is also tabulated.

Thermal properties include the coefficient of thermal expansion, specific heat, and thermal conductivity. Thermal properties vary as functions of temperature and crystal axis.

Other properties include: known laser lines, electro-optical coefficients, photo-elastic coefficients, relative dielectric constants and the velocity of sound.

4.2 Database Macros

Since the energy level table has received most of our attention, more macros reference data in the energy table level table than any other table. A series of 4 macros exists to determine possible wavelength transitions between energy levels. These macros differ only in the amount of information the user supplies. For example, one macro in the series provides the user with a list of hosts in the database which contain an energy level transition within the user-specified wavelength range for the selected active atom. Another macro in the series provides the user with all the wavelength transitions between 2 user selected manifolds for the selected active atom and laser material.

Table 3 shows an image of the screen which was generated when one of the macros in this series, ALTRANS, was executed. ALTRANS calculates all energy level differences and the corresponding wavelengths for the user selected active atom and laser material in the specified wavelength range. Input data entered at the requests are underlined. The macro begins by requesting the minimum and maximum wavelengths in micrometers. In this example, the wavelength range is .620 to .820

micrometers. The macro displayed the active atoms in the energy level table, the user was asked to select an active atom, and erbium was chosen. The macro displayed the hosts in the energy level table for Er, the user was asked to select a host, and $Y_3Al_5O_{12}$ was chosen. The macro computed energy level differences from the energy levels. Data for energy level differences corresponding to wavelengths beween .620 and .820 micrometers was saved. After sorting by wavelength, the upper laser level name and energy, the lower laser level name and energy, the energy difference, and the wavelength were printed to the screen. Two hundred and fifty-three additional transitions, which were identified by the macro, are not reproduced here. ALTRANS can be used, for example, to help a spectroscopist determine the transitions which generated a given line on an emission spectra.

Two macros assist the laser engineer in determining good candidates for sensitized materials. One macros finds identical or nearly identical energy level differences between pairs of manifolds for an active atom and a sensitizer in a common laser material. The other macro for sensitized materials creates an ASCII file containing data for use in the FORTRAN sensitizer transfer rate calculated from energy levels model. By judiciously interpreting the terms active atom and sensitizer, these macros may be used to investigate potential excited state absorption, up-conversion, in a laser material.

The last macro which utilizes data from the energy level table calculates energy centroids or partition functions for the selected active atom, host, and manifold at the specified temperature. Table 4 shows the screen image which was generated when macro CENTOID was executed. Here, the macro lists the active atoms in the energy level table and requests the user to select an active atom. Thulium was selected. The hosts in the tabler for Tm were listed and, as in the previous example, YAG was selected. The manifolds for Tm:YAG were listd and the $^3F_4$ level was selected. The user may calculate either the partition function for all energy levels in the manifold at a temperature which he will enter or the energy centroids between 25K and 350K in preprogrammed steps of 25K. The option to calculate the partition function was selected. At the next prompt, a temperature of 300K was entered. The partition function for each level in the manifold was calculated from the energies and degeneracies. The input parameters were echoed to the screen and the calculated energy centroid of the manifold at 300K was shown. Finally, the energy level energy, degeneracy, and partition function for each of the energy levels in the Tm:YAG $^3F_4$ manifold was displayed. The user has the opportunity to repeat the calculations at another temperature.

Additional macros have been created to retrieve data from the other tables. Three macros retrieve data from multiple tables. These three macros simply list data in the database for the specified active atom, host, or material name, as appropriate. One could, for example, retrieve all data in database LASERS for YAG by executing one of these macros. Another macro calculates the index of refraction from the Sellmeier coefficients for all optical axes for the selected material at the specified wavelength. Since most data is stored by chemical formula, a fifth macro allows the user to get the chemical formula for a given common name. A sixth macro creates an ASC II files with nonlinear materials data for use by a FORTRAN model which calculates the effective nonlinear coefficient.

In summary, macros easily retrieve data in a way that is useful to the laser engineer. Macros are developed on an as-needed basis.

Table 5 summarizes the current contents of database LASERS. For laser materials, each active atom-host combination is considered a separate entity. As indicated in Table 5, the energy level, nonlinear, known laser lines, and Sellmeier coefficients tables have received the most attention. The data in the nonlinear coefficients table represents approximately 150 nonlinear materials. The energy level table represents 176 laser materials. Most of the data in the energy level table comes from Kaminski[8] and the many publications by Morrison,[9-12] et.al. Since Kaminski's book was published almost 15 years ago, the Kaminski data is being selectively reviewed to update the table with more recent data. Absorption spectra and emission spectra continue to be added to database LASERS as spectroscopic samples become available. The data in the Sellmeier coefficients table represents 28 isotropic, uniaxial, and biaxial materials; Sellmeier coefficients continue to be added to the database on an as needed basis.

5.0 CONCLUSIONS

The physical parameters of materials, as well as laser models themselves, are required to design, test, and understand lasers. In some cases, relatively simple calculations using selected physical parameters of materials allow a laser researcher to gain insight to a laser process. A user-friendly, computerized, two-part database for laser, optical, and nonlinear materials has been created. Macros allows a laser engineer to easily access data from database LASERS. To date, a laser, optical, and nonlinear materials database containing spectra, tabulated data, and macros has been created. Spectra, tabulated data, and macros will be added to the database as needed.

6.0 ACKNOWLEDGMENTS

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Table 1 Summary of Existing Software

Efficiency calculations
- Flashlamp pumped laser absorption efficiency
- Laser diode pumped laser absorption efficiency
- User supplied spectra pumped laser absorption efficiency
- Radial distribution of absorbed energy
- Sensitizer transfer rate calculated from Dexter integrals

Electro-optical components
- Birefringent filter
- Fabry-Perot etalon
- Nonlinear elements

Laser amplifier and resonator models
- Pulse amplifier model
- Laser resonator model

Miscellaneous models
- Rb cell transmission
- Temperature distribution in the laser rod

Table 2: SAMPLE ABSORPTION SPECTRA HEADER

```
  11100 15  1 01NYAG8.SP PNYAG8 MS  .0000 U S1 012288 00.01   1   PROGRAM
PE-CONVERT VER  0.230
  USER MS  DATE & TIME  1988 01 28  14.56  53.08    1.8000    295K U
AU1 ND  100    0     0 YAG              0.500000 - 0.830000 .00010
FILE NAME ON PE-3600 = 001 NYAG8.SP       ON PC = 001NYAG8.SP
NO_POINTS  =  3301.    PTS    DATA_INTV = 0.000100 µm
MIN_LAMBDA =  0.500000 µm     MIN_DATA  =   0.
MAX_LAMBDA =  0.830000 µm     MAX_DATA  = 159180.
SCANSPEED  = .015      µm/min SLITWIDTH = 0.00020 µm ITA = 0.
     RESP  =  0.5      sec        ISMS  = 0.         DATE = 88/01/22
     INST  = 509.                    ? = 0.

THIS IS A Nd:YAG SAMPLE FOUND IN CHUCK'S LAB.  ASSUMED 1% CONCENTRATION, SAMPLE
1.8 MM THICK. STORM
CHANGED 0 AU BY MARK STORM ON 3/4/88.  HEADER DONE BY HAND.
Nd:YAG, 1%ND, 1.88MM, HIGH RES FINAL SCAN, STORM
 EOH.      (1X,F11.4)
  3301.
   1429.9563        = DATA VALUE AT 0.500000 µm
   1437.0537
   1372.1863
   1262.9418
   1348.7021
   1140.5082
   1260.2499
   1246.8193
```

Table 3: MACRO ALTRANS

```
R> run altrans.mac

     ENTER MINIMUM WAVELENGTH OF INTEREST IN MICRONS. .6200
     ENTER MAXIMUM WAVELENGTH OF INTEREST IN MICRONS. .8200

     ATOMNAME Number of Occurrences
     ------------------------------
           Dy               3
           Er              15
           Eu               2
           Ho              12
           Nd              57
           Pr               5
           Sm               1
           Tm               7
           U                3
           Yb               3

     ENTER ACTIVE ATOM NAME. er
```

Table 3: MACRO ALTRANS (Continued)

HOST	Number of Occurrences
BaY_2F_8	1
CaF_2-YF_3	1
$CaWO_4$	1
$Er_3Al_5O_{12}$	1
$KGd(WO_4)^2$	1
$KY(WO_4)^2$	1
LaF_3	1
$LiNbO_3$	1
$LiYF_4$	1
$Lu_3Al_5O_{12}$	1
$Y_3Al_5O_{12}$	1
$Y_3Ga_5O_{12}$	1
$YAlO_3$	1
YVO_4	1

ENTER HOST NAME. y3al5o12

NAME ULL = Upper Laser Level Name
ENGYULL = Upper Laser Level Energy in inverse centimeters
NAME LLL = Lower Laser Level Name
ENGYLLL = Lower Laser Level Energy in inverse centimeters
ENGY DIFF = (Upper-Lower) Laser Level Energy in inverse centimeters
WAVELEN = Wavelength in microns

NAME ULL	ENGYULL	NAME LLL	ENGYLLL	ENGY DIF	WAVELEN
2H9/2	24784.	4I9/2	12577.	12207.	0.819202
2H11/2	19093.	4I13/2	6885.	12208.	0.819135
4F3/2	22585.	4I11/2	10373.	12212.	0.818867
4F3/2	22585.	4I11/2	10362.	12223.	0.81813
4I9/2	12303.	4I15/2	79.	12224.	0.818063
2H11/2	19114.	4I13/2	6885.	12229.	0.817728
2H9/2	24765.	4I9/2	12527.	12238.	0.817127
4I9/2	12765.	4I15/2	526.	12239.	0.81706
4F3/2	22659.	4I11/2	10419.	12240.	0.816993
4I9/2	12303.	4I15/2	61.	12242.	0.81686
4F3/2	22659.	4I11/2	10414.	12245.	0.81666
2H9/2	24784.	4I9/2	12527.	12257.	0.81586
2H11/2	19151.	4I13/2	6885.	12266.	0.815262
2H11/2	19093.	4I13/2	6823.	12270.	0.814996
2H9/2	24576.	4I11/2	12303.	12273.	0.814797

***** 253 LINES WERE DELETED FROM THIS EXAMPLE *****

Table 4: Macro CENTOID

```
R> run centoid.mac

     ATOMNAME Number of Occurrences
     -------- --------------------
     Dy                        3
     Er                       15
     Eu                        2
     Ho                       12
     Nd                       57
     Pr                        5
     Sm                        1
     Tm                        7
     U                         3
     Yb                        3

Enter active atom name. tm

     HOST            Number of Occurrences
     --------------- --------------------
     CaWO4                             1
     GdAlO3                            1
     LiYF4                             1
     Y3Al5O12                          1
     Y3Ga5O12                          1
     YAlO3                             1

 ENTER HOST NAME. y3al5o12

     ELEVNAME        Number of Occurrences
     --------------- --------------------
     1D2                               4
     1G4                               6
     1I6                               7
     3F2                               4
     3F3                               7
     3F4                               9
     3H4                               8
     3H5                              11
     3H6                               9
     3P0                               1
     3P1                               3
     3P2                               4

ENTER MANIFOLD NAME. 3f4

You have two options:
1) Partition func. and energy centroid at user specified temperatures
2) Energy centroid at preprogrammed temperatures (25 to 350 K in steps of 25
   degrees)
ENTER OPTION 1 OR 2. 1
ENTER TEMPERATURE IN KELVIN. 300.
```

Table 4: MACRO CENTOID (Continued)

ATOM
TM
HOST
$Y_3AL_5O_{12}$
MANIFOLD NAME
$^3F_4$
TEMPERATURE 300
ENERGY LEVELS, DEGENERACY, AND PARTITION FUNCTION FOR THE MANIFOLD
ENERGY CENTROID IN INVERSE CENTIMETERS. 5732.037
ENGY = ENERGY IN INVERSE CENTIMETERS
ECY
PARTION = PARTITION FUNCTION

ENGY	G	PARTION
5556.	1	.453273
5736.	1	.191127
5808.	1	.135303
5907.	1	.084146
6041.	1	.044243
6108.	1	.032081
6170.	1	.023827
6224.	1	.018389
6233.	1	.017612

ANOTHER TEMPERATURE (Y OR N)? n

Table 5: CURRENT CONTENTS OF DATABASE LASERS

Table	Rows
Absorption/emission spectra	48
Chemical names and formulas	38
Conductivity	114
Damage Threshold	41
Density	126
Dn/DT	50
Electro-optical coeff.	8
Energy Level	7908
Thermal expansion coeff.	129
Known laser lines	928
Linewidth	45
Lifetime	26
Nonlinear coeff.	486
Photo-optical coeff.	9
Physical parameters	20
Relative dielectric coeff.	47
Sellmeier coeff.	58
Specific heat	113
Transmission range	77
Velocity of sound	8
Yield strength	2
Young's modulus	36