*NIST Standard Reference Database 30*

# NIST Structural Ceramics Database

Version 2.0

Users' Guide

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## ACKNOWLEDGMENT

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# I. INTRODUCTION

The NIST Structural Ceramics Database (SCD) is a materials properties database designed as a user-friendly system for use on personal computers. Users of the SCD may search easily for properties of a given material or identify materials that have specified properties.

The SCD project was designed at NIST under funding from the Gas Research Institute (GRI) and is intended to reduce the technology transfer barriers impeding the application of advanced structural ceramics in industry. These materials hold particular promise for improving the durability and efficiency of gas-fueled high temperature components, such as heat-exchangers and recuperators. However, these materials are complex and evolving rapidly.

The Structural Ceramics Database: (1) provides quick and efficient access to critical data which strengthens the link between the development of new materials in research laboratories and the application of those materials in industry, (2) provides consistent treatment of data which may improve quality control and product reliability, and (3) enhances the continuity of research and development programs.

The focus for the first version of the database was on silicon carbides and silicon nitrides. In Version 2.0 of the SCD, the scope has been expanded to include some oxides (alumina, beryllia, and zirconia) as well as aluminum nitride and boron nitride. Version 2.0 of the Structural Ceramics Database includes: thermal properties (conductivity, expansion, diffusivity, specific heat, and shock resistance); mechanical properties (bulk modulus, elastic modulus, shear modulus, Weibull modulus, Poisson's ratio, compressive, flexural, and tensile strengths, Knoop hardness, Vickers hardness, fracture toughness, fracture energy, creep exponent, creep rate, crack growth exponent, and creep activation energy); and corrosion and oxidation properties (oxidation rate, oxidation activation energy, and molecular oxygen diffusivity). Chemical composition (including sintering aids and impurities) and physical properties (such as density, porosity, and grain size) were included as part of the material specification information. Complete bibliographic references to the data are available.

Data for the SCD were obtained from publicly available technical literature such as professional journals and technical reports to Federal agencies.

# II. SYSTEM REQUIREMENTS AND INSTALLATION[1]

## SYSTEM REQUIREMENTS

- An operating system compatible with MS-DOS® version 2.1 or higher
- At least an enhanced graphics adapter (EGA) with appropriate color monitor
- At least 512 kilobytes of random access memory (RAM)
- At least 4 megabytes of hard disk storage and one floppy disk drive for reading the installation disks

The program can be made available on any of the following disk formats:

- High density 5¼ inch diskettes (1.2 megabytes) (4 diskettes)
- High density 3½ inch diskettes (1.4 megabytes) (4 diskettes)
- Low density 3½ inch diskettes (720 kilobytes) (8 diskettes)

## INSTALLATION INSTRUCTIONS

To install the database, place diskette number 1 in drive A (substitute your drive letter if different), and enter the following:

**A:**
**INSTALL**

Instructions will be provided and you will be prompted for each diskette.

***Special Note with Caution***

Personal computer databases, in general, make extensive use of the hard disk drive in order to access required information. Since reading the hard drive is a relatively slow process, it often affects one's perception of system performance. To improve performance, add these lines to your CONFIG.SYS file:

Files = 20
Buffers = 30

(Remember to reboot your computer after editing the **CONFIG.SYS** file.)

Please note that by setting different values for the BUFFERS command and running the SCD, you will be able to find the optimal number of buffers for your system. It is *especially important* to remember that if you modify the number of buffers for the purpose of improving the performance of the SCD, the performance of other applications software may be affected.

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[1]Certain commercial names are identified in this document for the purpose of clarity in the presentation. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology.

# III. USE OF THE STRUCTURAL CERAMICS DATABASE

## OVERVIEW

In using the Structural Ceramics Database, choices are made by menus, fill-in forms, and single keystroke commands. Each of these three features will be examined in this section. A typical session is shown in Appendix A.

Most use of the database is self-evident, that is, the screens are self-guiding. Help screens should clarify any ambiguity or problems. Three keys are used throughout that will aid ease of use:

| | |
|---|---|
| **F1** | Help |
| **F2** | Select an entry for a property or characteristic |
| **F9** | Accept current screen and continue |

An exhaustive survey of the contents of these screens is beyond the scope of this users' guide. This introduction provides an overview; and exploring the screens prior to serious use of the database is easy and encouraged.

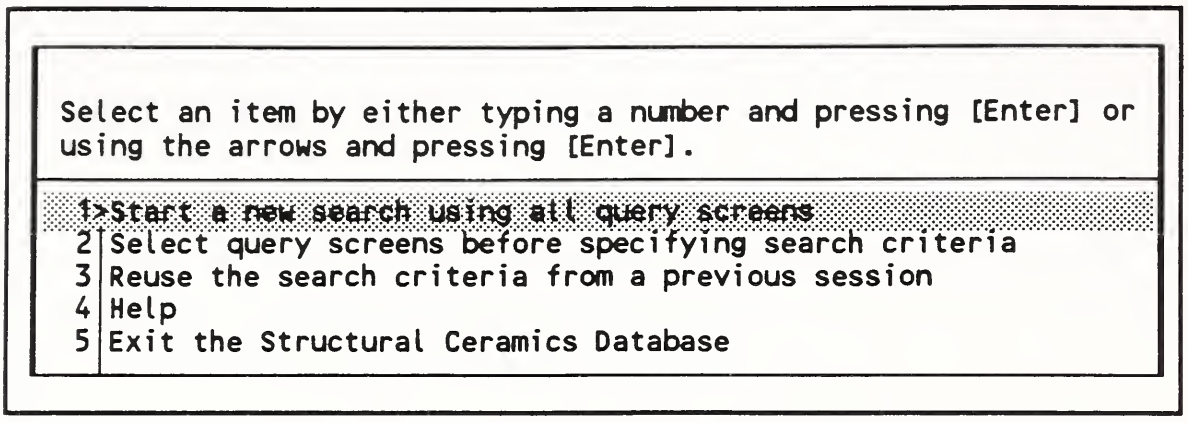
## STARTING THE DATABASE

To begin the program: 1) change the directory to the one containing the application software (which is by default \SCD_DB); 2) type SCD; and 3) press **ENTER**.

C:\>**cd \SCD_DB**
C:\SCD_DB>**SCD** **ENTER**

## USING THE MAIN MENU

The software will run though its initialization process, display the title and disclaimer screens, and present the menu shown below.




A choice from this menu is made in either of two ways: (1) move the highlight bar using the cursor (or ↑↓) keys down to the item of interest and then press **ENTER**, or (2) type the number of the item and then press **ENTER**. There are on-screen directions for this procedure as well as online help, if needed.

Searches are done by filling in a sequence of query specification screens with desired search criteria. Choices 1, 2, and 3 of the Main Menu cover different possible uses.

1. **Start a new search using all query screens** — Choice 1 is for the situation where most or all query screens may be needed to construct a query. The system will display each screen in turn.

2. **Select query screens before specifying search criteria** — Choice 2 is for the case where only certain screens will be needed for the intended search. The database first gives a list of possible screens. User selects from individual query screens.

   A useful rule when setting up a query is to avoid overconstraining the search. For example, if every prompt on every screen is filled in, it is highly likely that no records will be retrieved satisfying all the criteria. Start with a minimal specification. If too many records are retrieved, go back and refine the criteria (Item 3, Main Menu) until the set of records is satisfactory.

3. **Reuse the search criteria from a previous session** — Choice 3 of the menu allows one to reuse a search specification that had been saved previously. When 3 is selected, each stored specification is displayed in summary form and may be reviewed and ignored, discarded, or chosen. How specifications may be saved is discussed later in this guide.

4. **Help** — When choice 4 is selected, general help for using the Structural Ceramics Database is displayed. You may page through the text using the **PGUP** and **PGDN** keys and return to the menu by pressing the **ESC** key. Elsewhere in the SCD, help is available if "[F1] Help" appears in the lower portion of the screen. Pressing the single key, **F1**, requests help.

5. **Exit** — If one wishes to exit the database, choice 5 should be used.

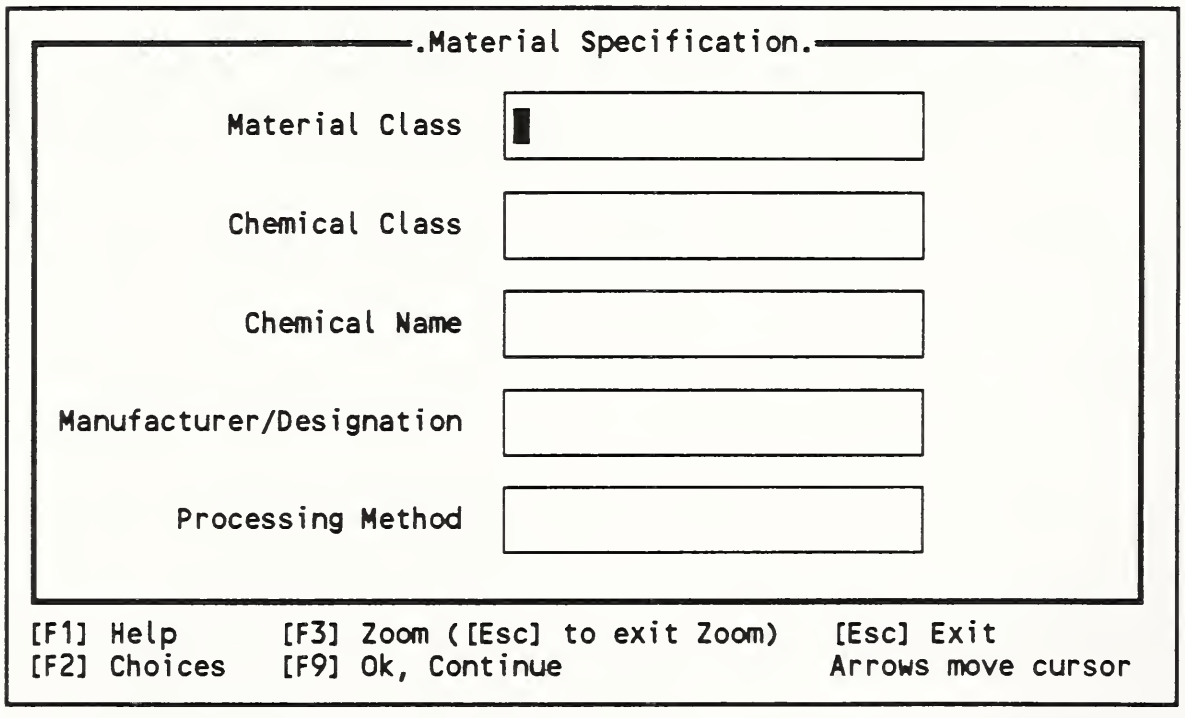
## SPECIFYING QUERIES

Query specifications are divided into seven query screens:

1. Material Specification
2. Chemical and Physical Characteristics
3. Thermal Properties
4. Elastic Properties
5. Strength Properties
6. Creep Properties
7. Corrosion and Oxidation Properties

Each of these screens has several additional levels of choices that can be specified. Let's take a closer look at how a query screen is used.

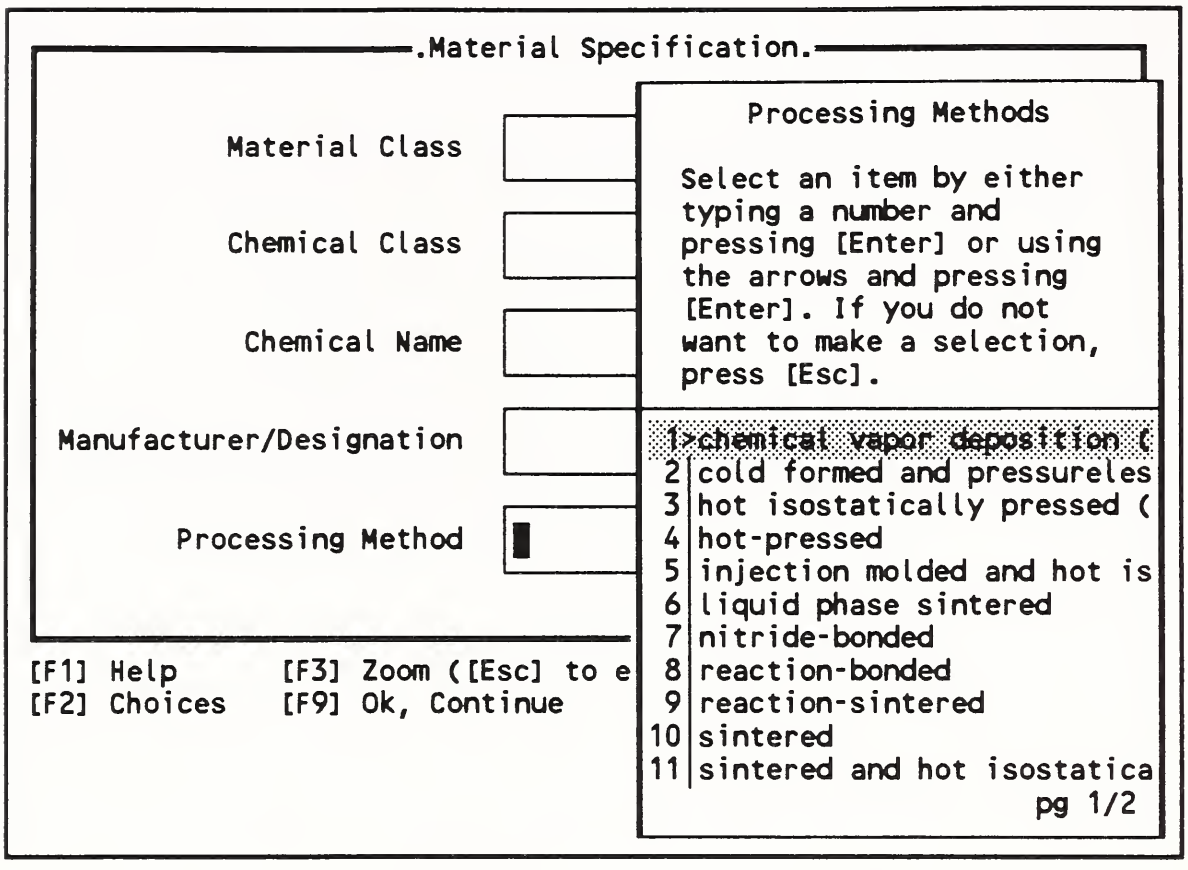
For this example, the user has chosen item 2 from the initial menu, has selected "Material Specification" from the list of query screens, and is presented immediately with the screen shown below.



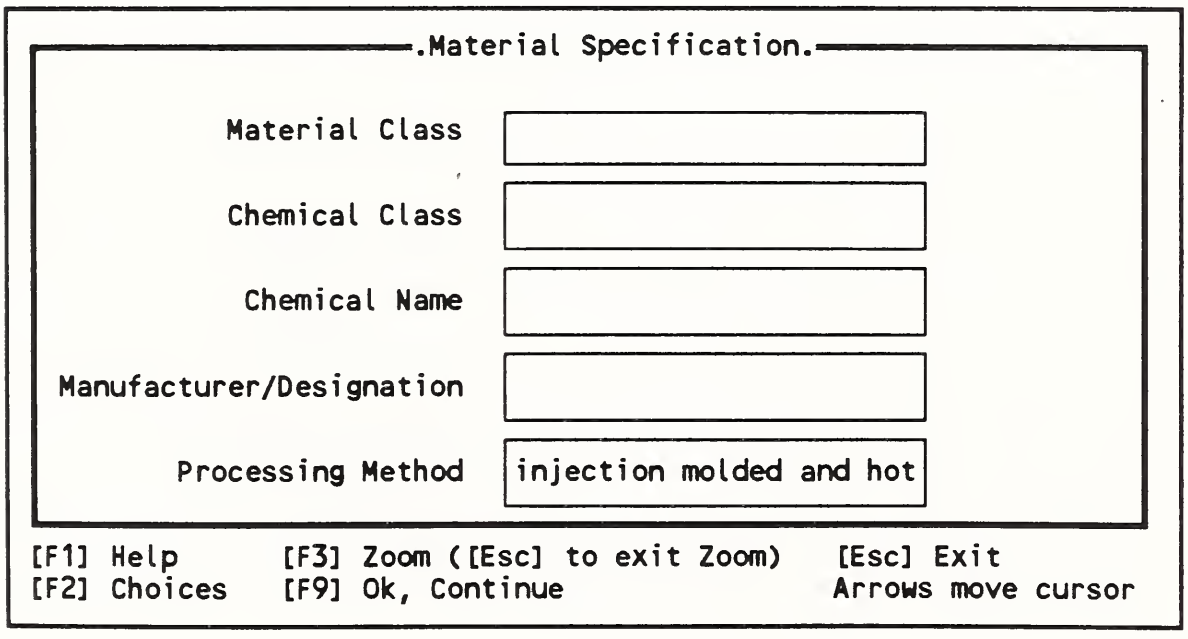

The structure of the Material Specification screen is representative of all other query screens. There are prompts which, in the figure, are the rectangular boxes with associated titles, a cursor resting in the prompt box (in this figure, the cursor is depicted by a small black rectangle, as found at the Material Class prompt), and single keystroke commands listed at the very bottom of the screen.

In order to reduce frustration and curb typographical errors, the user does not type directly into the prompt area. Instead, selections are made from a menu of appropriate choices. Action is initiated by placing the cursor at the appropriate prompt and pressing the F2 key.

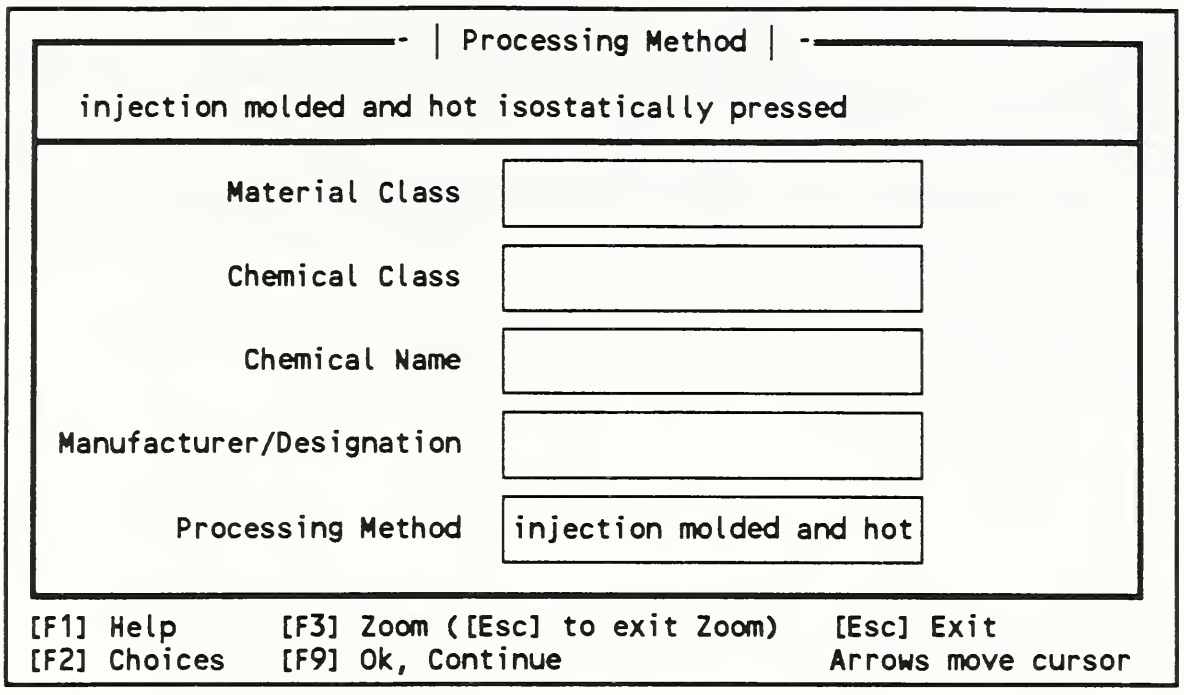
For example, if the cursor were positioned on the Processing Method and the F2 key were pressed, a menu listing the processing methods available in the database would appear as follows.




The user may now select a processing method from the list and it will appear in the prompt box on the Material Specification screen. If "5 injection molded and hot is" is selected, the screen will be as follows.

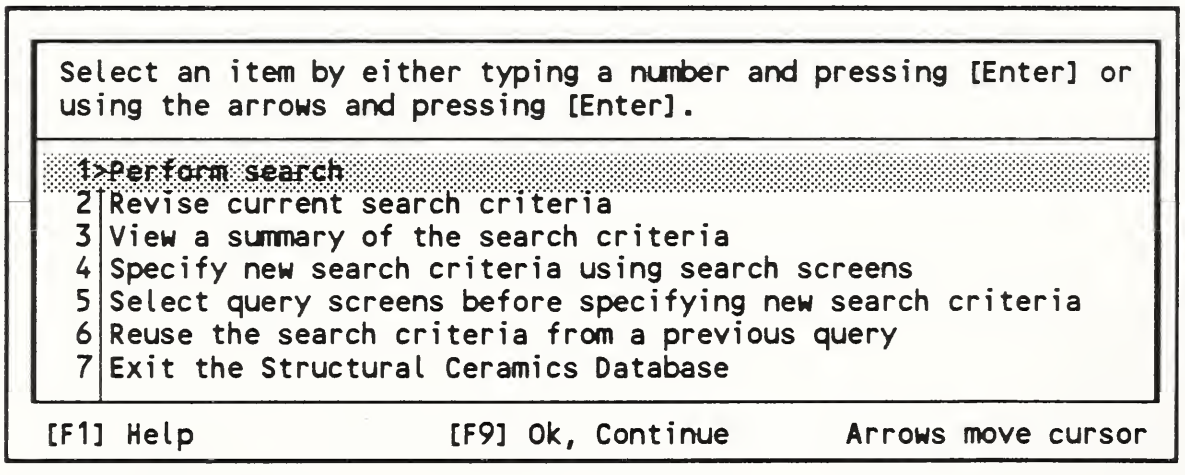


Text for some of the processing methods has been truncated in order to fit into the window. The complete text for the processing method can be displayed at the top of the screen by using the "[F3] Zoom" option as shown on this screen.




Pressing **ESC** will remove the Zoom box for Processing Method.

When all needed prompts are filled in on a query screen, press **F9** to move on to the next step. In this case, it is assumed that Processing Method is the only prompt being specified and Material Specification is the only query screen used. **F9** is pressed and a menu is displayed listing the next options.



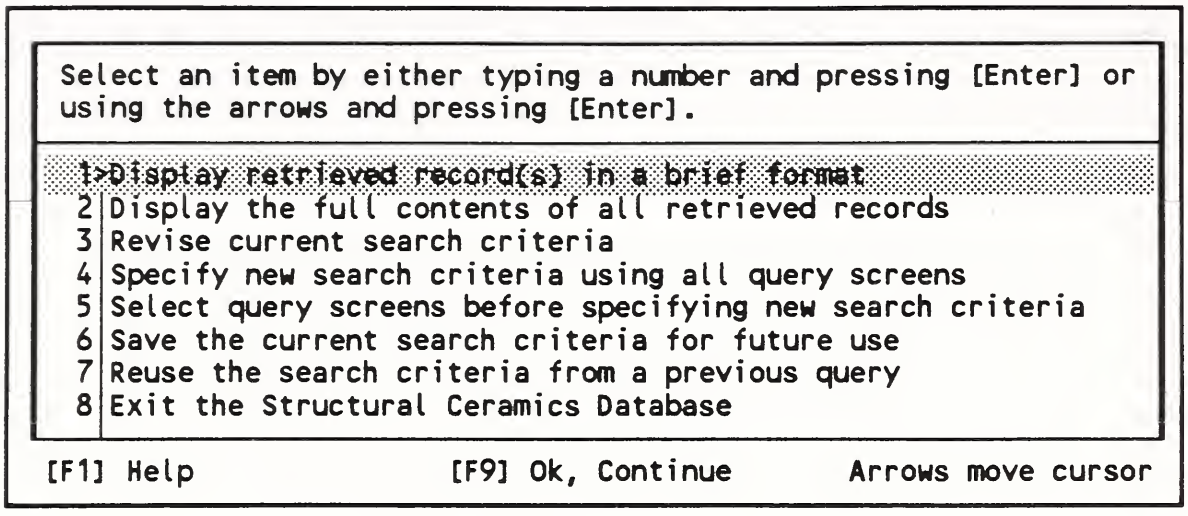

1 starts the search.

2 provides an opportunity to revise the specified criteria. After it is chosen, the selected query screens are presented for revision.

3 displays a summary report of the search criteria.

4, 5, 6, and 7 have the same meanings as were assigned to them earlier (page 4).

Assuming option 1 is selected, the search begins. When the search is finished, the number of records matching the search criteria is reported. Another menu then appears:




1 displays the retrieved records in a short format for rapid review. The user may select records from this list for full content display.

2 displays the complete contents of all retrieved records.

3, 4, 5, 7, and 8 have been discussed.

6 allows the user to save the current search specification so that it can be used at some future time.

## DISPLAYING SEARCH RESULTS

Item 1 tells the software to display the retrieved records in a brief format. Records may then be selected from the list for full content display. An example of this brief display appears as follows:

**Translation Table for Property Codes Used in the Brief Display**

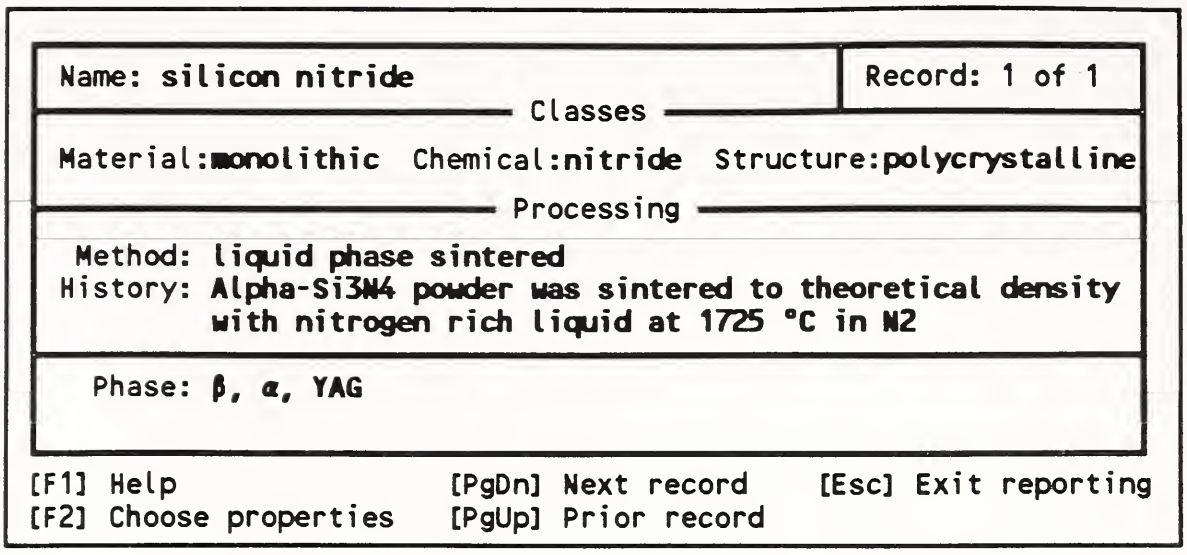
| | | |
|---|---|---|
| Bulk Modulus | Flexural Strength | Specific Heat |
| Creep Activation Energy | Fracture Toughness | Shear Modulus |
| Creep Exponent | Knoop Hardness | Thermal Conductivity |
| Crack Growth Exponent | Oxidation Activation Energy | Thermal Diffusivity |
| Creep Rate | Molecular Oxygen Diffusivity | Thermal Expansion |
| Compressive Strength | Oxidation Rate | Tensile Strength |
| Elastic Modulus | Poissons Ratio | Vickers Hardness |
| Fracture Energy | Thermal Shock Damage | Weibull Modulus |

Items in this list may be selected for full record display. Select the items by either typing a number and pressing [Enter] or using the arrows and pressing [Enter]. Remember to press [F9] when you are done making selections.

| | Material Designation | Properties Available |
|---|---|---|
| 1> | silicon carbide (Carborundum Company Hexoloy SA) | FS FT |
| 2 | silicon carbide (Sohio Hexoloy SA) | EM FS TE WM |
| 3 | silicon nitride (GTE PY6) | EM FS TE WM |
| 4 | silicon nitride (In house) | EM FS FT VH |
| 5 | silicon nitride (Norton/TRW XL-144) | EM FS TE WM |
| 6 | silicon nitride (United Techonologies CVD Si3N4) | OA OR |

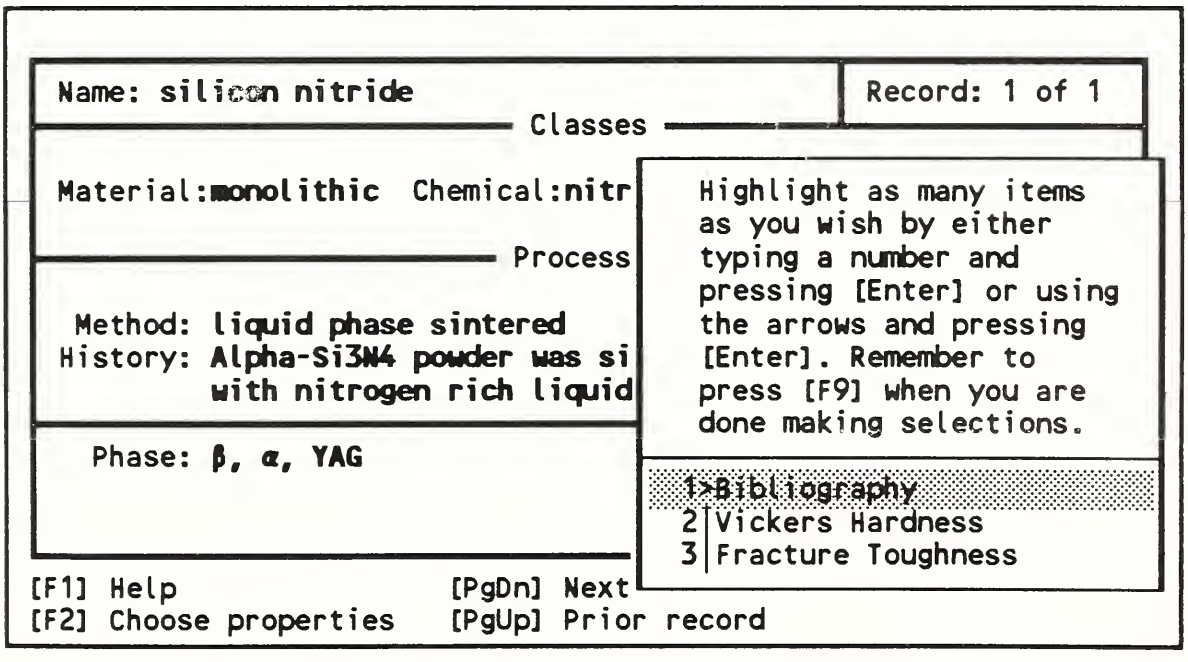
Item 2 tells the system to begin displaying the full contents of the retrieved records using the specified criteria. Since there is generally more information available for a given record than can fit on a single screen, two types of screens are used: material specification and property measurements.

The material specification reporting screen appears as follows:




The record counter is located in the upper right corner of the display. This is helpful for navigating among records. The **PGDN** and **PGUP** single keystroke commands, as listed at the bottom of the screen, are used for changing records. **ESC** will return the user to the menu that was used to enter the reporting mode.

Pressing **F2** will supply a menu of properties. Any properties that have been measured for this material/record will appear in the list and any number of them may be selected. For example, if **F2** were pressed for the above record, the screen would appear as follows:




The menu shows that a bibliographic citation is available for the record as well as property measurements for Vickers Hardness and Fracture Toughness. To view the additional information, highlight the items of interest and press **F9**.

If, for example, Bibliography and Vickers Hardness were selected and **F9** is pressed, the bibliographic citation would be displayed immediately.

```
Name: silicon nitride                                  Record: 1 of 1
                              Bibliography

Chakraborty, D.; Mukhopadhyay, A.K.; Mukerji, J. Influence of
thermal quenching on surface fracture toughness and microhardness
of Si3N4, SiA1ON and SiC Rev. Int. Hautes Temp. Refract. Vol. 22,
105-113; 1985.

Use arrow keys to pan the display since more information may be available.

[F1] Help                [PgDn] Next property     [Esc] Exit reporting
[F2] Choose properties   [PgUp] Prior property    [Home] Return to description
```

To view Vickers Hardness measurements in the previous figure, the **PGDN** key is pressed. The data are displayed as follows:

```
Name: silicon nitride                                  Record: 1 of 1
                              Vicker's Hardness

  Temperature °C        Vickers Hardness GPa        Number of Quenches
        22                    16.27                       0
        22                    16.18                       1
        22                    16.18                       2
        22                    16.37                       3
        22                    15.69                       4
        22                    16.47                       10
        22                    16.37                       15
        22                    15.98                       20
    Method: Vickers indentation
     Notes: Leitz miniload hardness tester used
Preparation: Samples mounted in resin, ground and mechanically polished
             with diamond paste, quenching temperature was 1300°C
  Cautions: Quenching temperature was 1300°C, and data have been
             digitized from Figure 7 in paper
Comments: Quenching method-specimen was heated in platinum tube furnac

Use arrow keys to pan the display since more information may be available.

[F1] Help                [PgDn] Next property     [Esc] Exit reporting
[F2] Choose properties   [PgUp] Prior property    [Home] Return to description
```

One can move among the property displays by using the **PGDN** and **PGUP** keys and can return to the material specification screen by pressing **HOME**. The **F8** key is used to request a plot of the property as a function of temperature.

# IV. REFERENCES


1. Property Database for Gas-Fired Applications of Ceramics – R. G. Munro and C. R. Hubbard. Ceramic Bulletin **69**, 1498 (1989).

2. The Structural Ceramics Database: Technical Foundations – R. G. Munro, F. Y. Hwang, and C. R. Hubbard. NIST J. of Research **94**, 37 (1989).

3. Strengths and Deficiencies in Published Advanced Ceramics Data – R. G. Munro, E. F. Begley, and T. L. Baker. Ceramic Bulletin **69**, 1498 (1990).

4. Materials Property Database Requirements for Gas-Fueled Ceramic Heat Exchangers – R. G. Munro and E. F. Begley. Second International Symposium on Computerization of Materials Property Data, Issues in Data Exchange. J. G. Kaufman and G. S. Glazman, eds. (ASTM, Philadelphia, PA 1991).

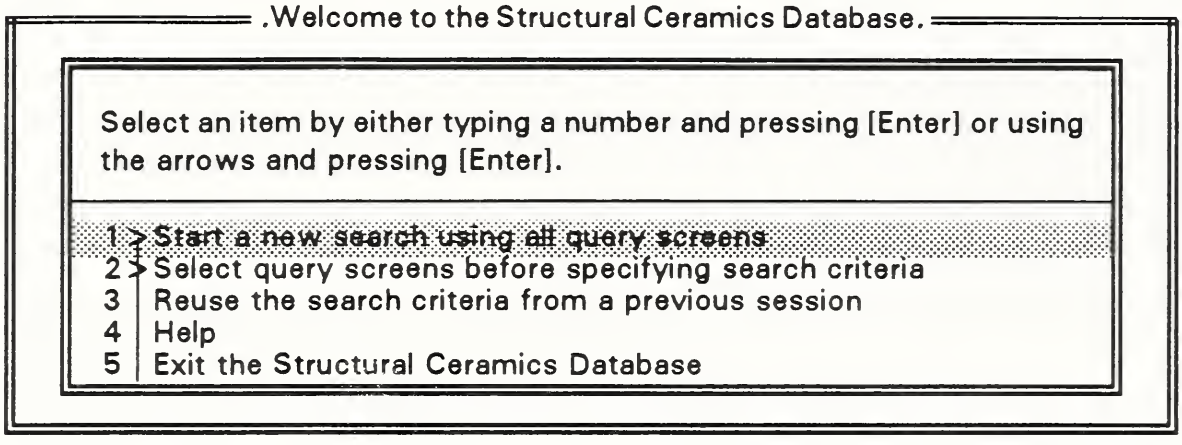
# Appendix A

## TYPICAL SESSION

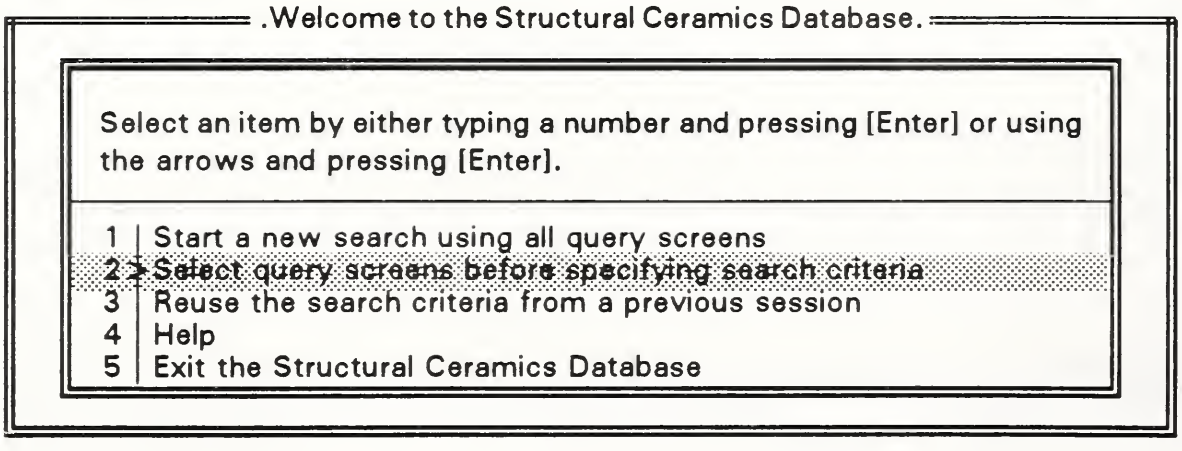
This appendix contains screen mockups of a session with the Structural Ceramics Database. While the actual database makes use of color for certain system features, the typographical restrictions of this documentation force some simulations. Gray highlighting will serve as the blue highlight bar found in the actual menus.

To set the context for the session, the user is looking for a silicon nitride in the $\beta$ phase with yttrium oxide (Y2O3) used as a sintering aid. Furthermore, the flexural strength of the material must equal or exceed 300 MPa and have a thermal expansion of less than or equal to 4.0 10^-6 C^-1.

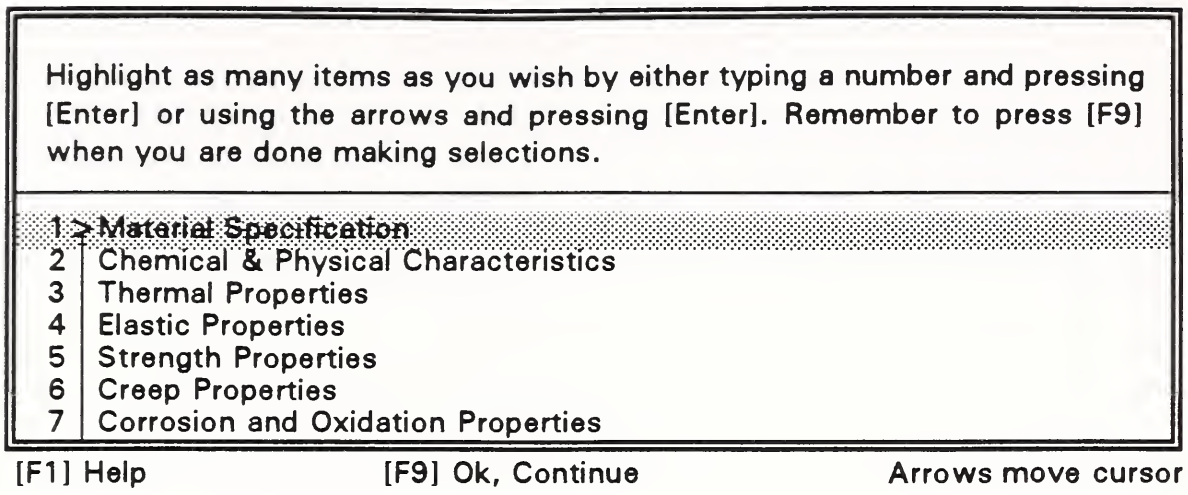
*To begin the session, change to the appropriate directory, by default C:\SCD_DB, and type SCD. Title and disclaimer screens will appear, followed by this welcome menu.*



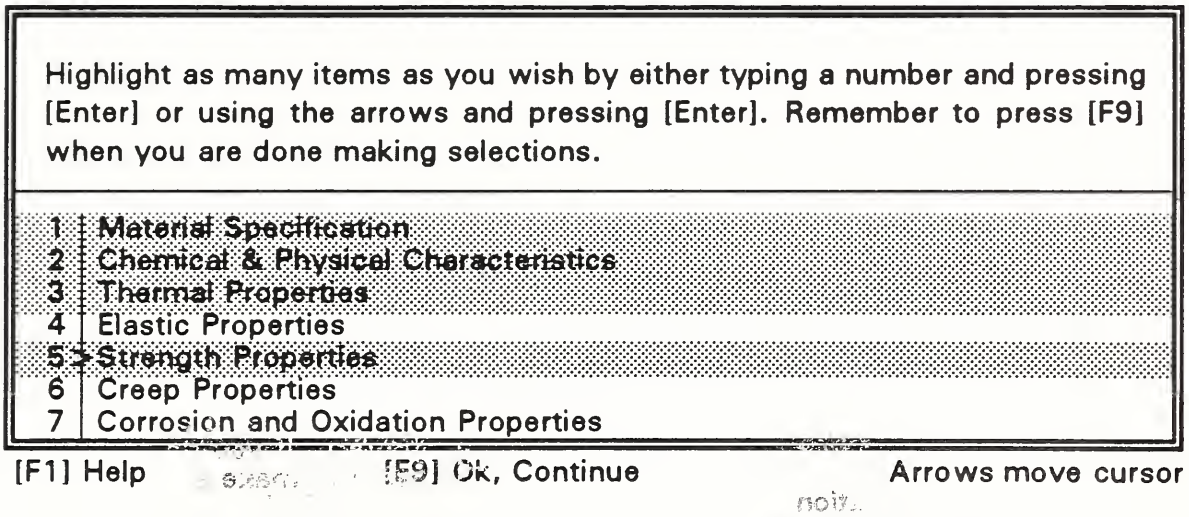

*For this example, the user wishes to select the screens to be used for specifying the search criteria, so the highlight bar is moved to item 2.*



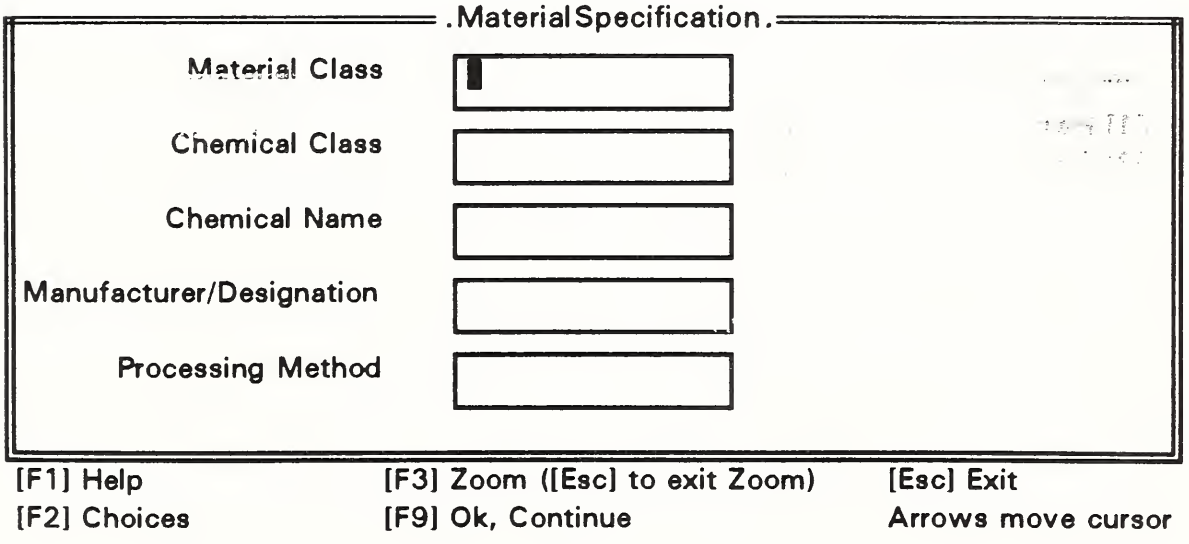
*F9 is then pressed and the menu of screens is presented.*



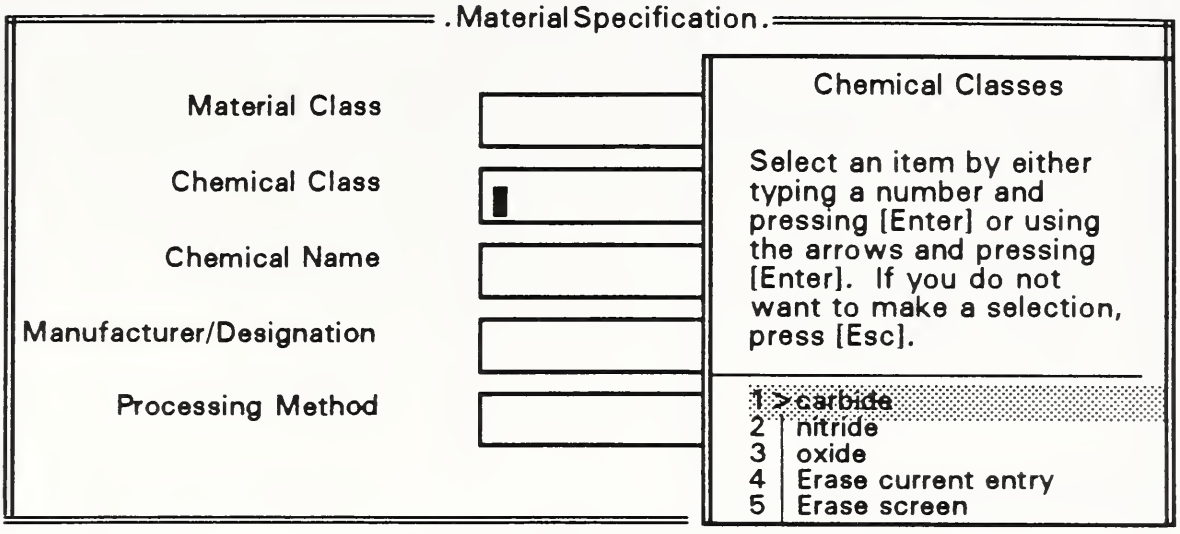

*Items 1, 2, 3, and 5 are selected by using the arrow key to move to them and then pressing **ENTER** at each one.*



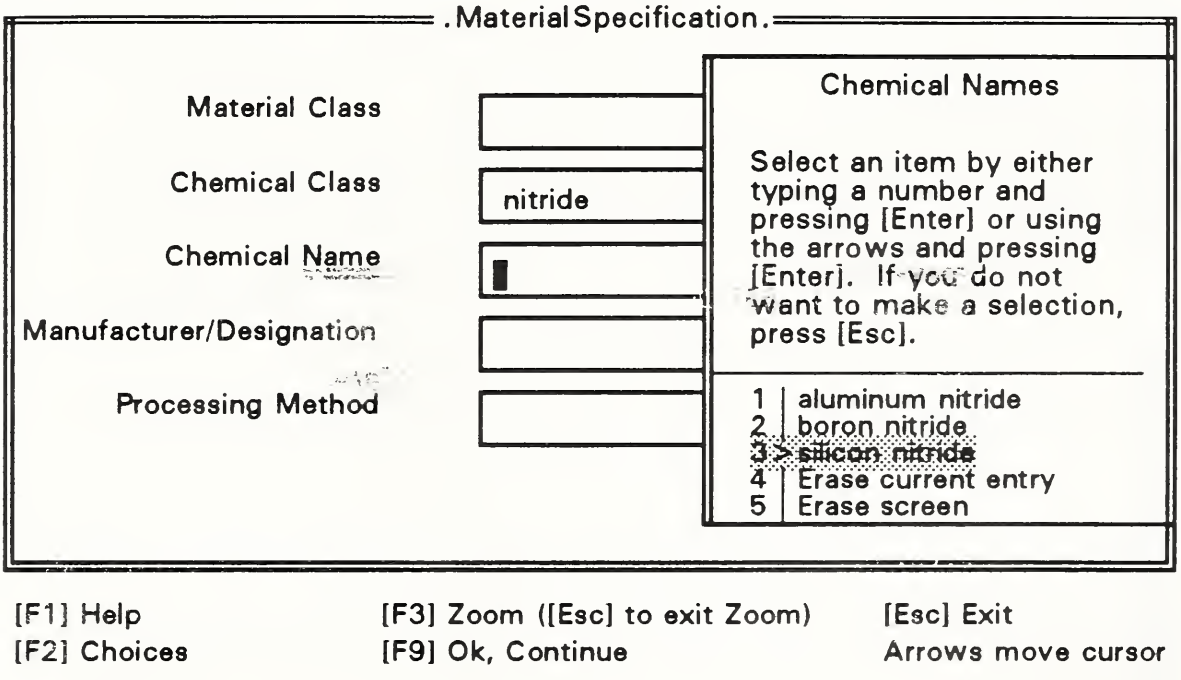

*F9 is pressed and the first query screen, Material Specification, is displayed.*



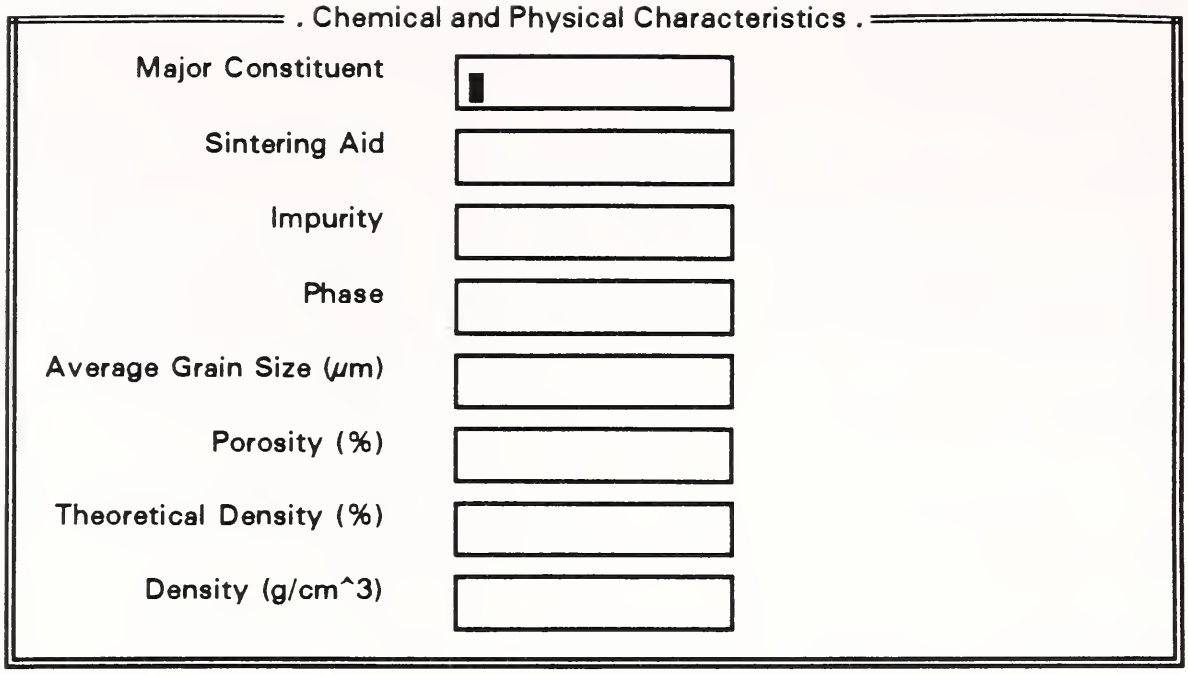
*The cursor is placed on the Chemical Class prompt and **F2** is pressed.*



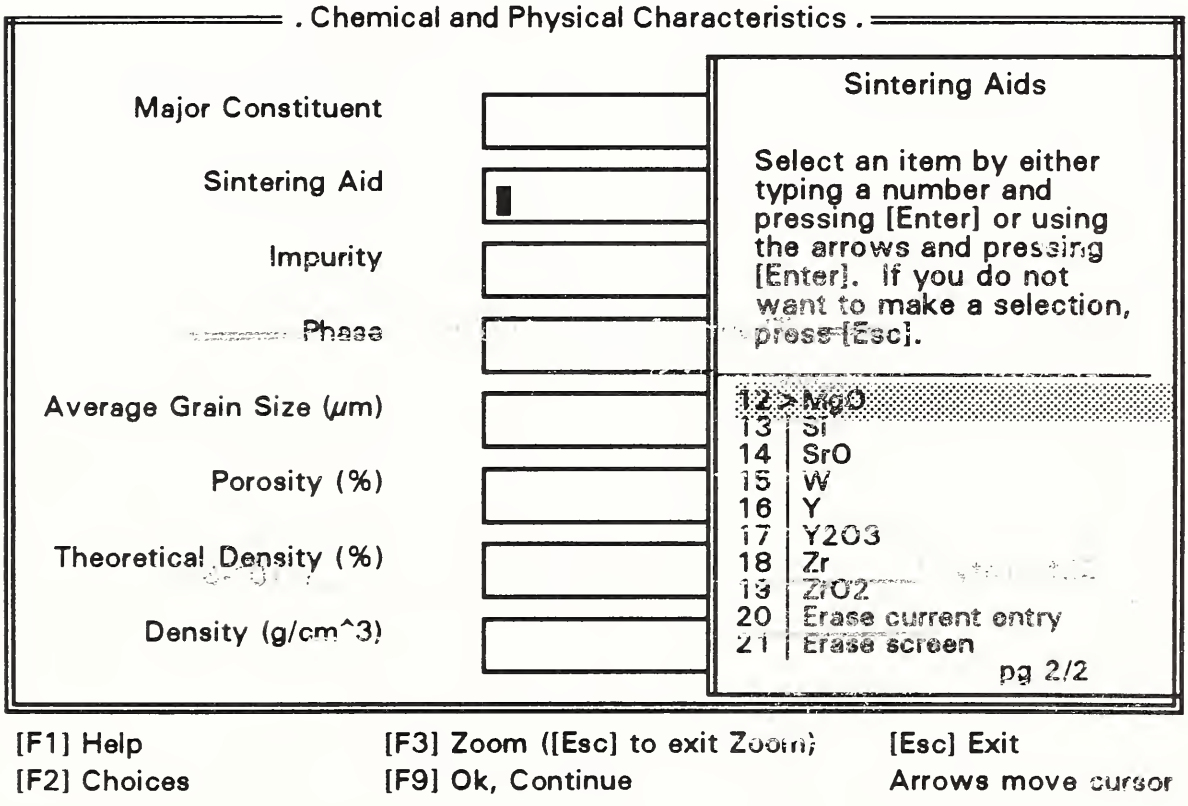

*The user selects "nitride" by moving the light bar there or pressing 2 and then pressing **ENTER**. Then the cursor is moved to the Chemical Name prompt and **F2** is pressed.*




*Silicon nitride is selected and **F9** is pressed, indicating that all items for this screen have been selected. Once **F9** is pressed the next screen, Chemical and Physical Characteristics, appears.*




*Using the ↓, the cursor is positioned on the Sintering Aid prompt, **F2** is pressed, and a menu of sintering aids is presented.*




*Use the **PGDN** key to display page 2 of the items list in the sintering aids window.*

*Y2O3 is selected by moving the lightbar with the ↓ and pressing* ***ENTER****. Then the cursor is positioned on the Phase prompt, and* ***F2*** *is pressed for a list of phases.*

. Chemical and Physical Characteristics .

| | |
|---|---|
| Major Constituent | |
| Sintering Aid | Y2O3 |
| Impurity | |
| Phase | |
| Average Grain Size (μm) | |
| Porosity (%) | |
| Theoretical Density (%) | |
| Density (g/cm^3) | |

Phases

Select an item by either typing a number and pressing [Enter] or using the arrows and pressing [Enter]. If you do not want to make a selection, press [Esc].

| | |
|---|---|
| 1 | >alpha |
| 2 | alpha (4H) |
| 3 | alpha (6H) |
| 4 | alpha (15R) |
| 5 | beta |
| 6 | beta (3C) |
| 7 | beta-Si3N4 |
| 8 | BN |
| 9 | FeWSi |
| 10 | H-phase |
| 11 | hexagonal 4H |

pg 1/2

[F1] Help [F3] Zoom ([Esc] to exit Zoom) [Esc] Exit
[F2] Choices [F9] Ok, Continue Arrows move cursor

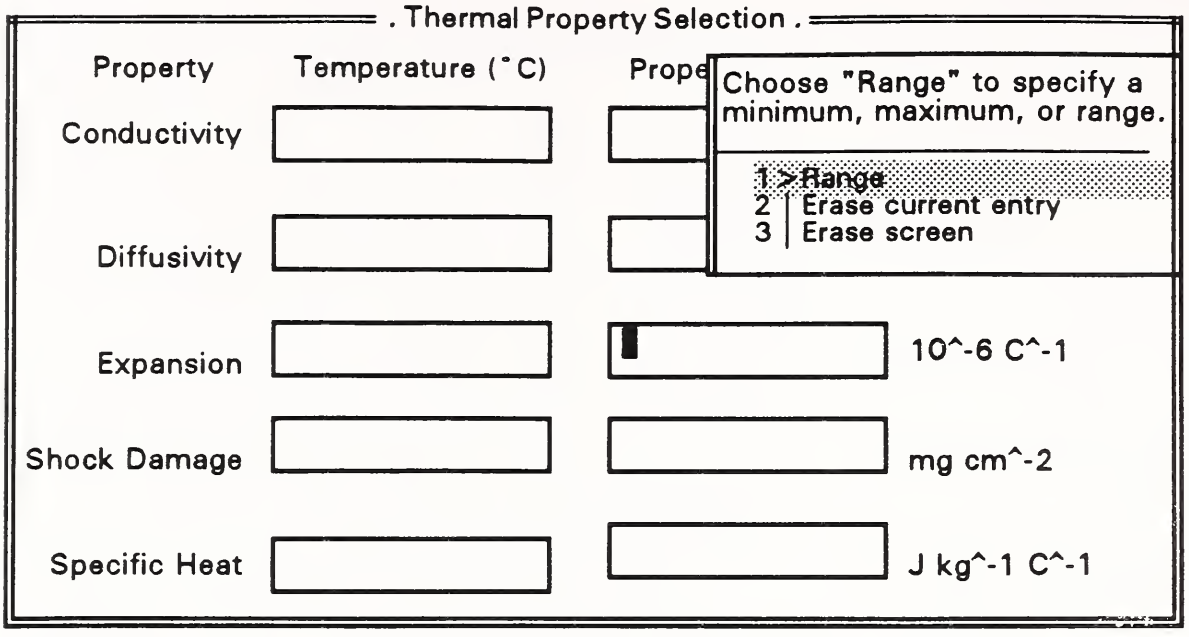
*Beta is chosen from the list by moving the lightbar to beta and pressing* ***ENTER****. Since all entries have been made for this screen, the* ***F9*** *key is pressed to continue with the next step, which is to constrain the thermal expansion.*

. Thermal Property Selection .

| Property | Temperature (°C) | Property Value | |
|---|---|---|---|
| Conductivity | | | W m^-1 C^-1 |
| Diffusivity | | | 10^-6 m^2 s^-1 |
| Expansion | | | 10^-6 C^-1 |
| Shock Damage | | | mg cm^-2 |
| Specific Heat | | | J kg^-1 C^-1 |

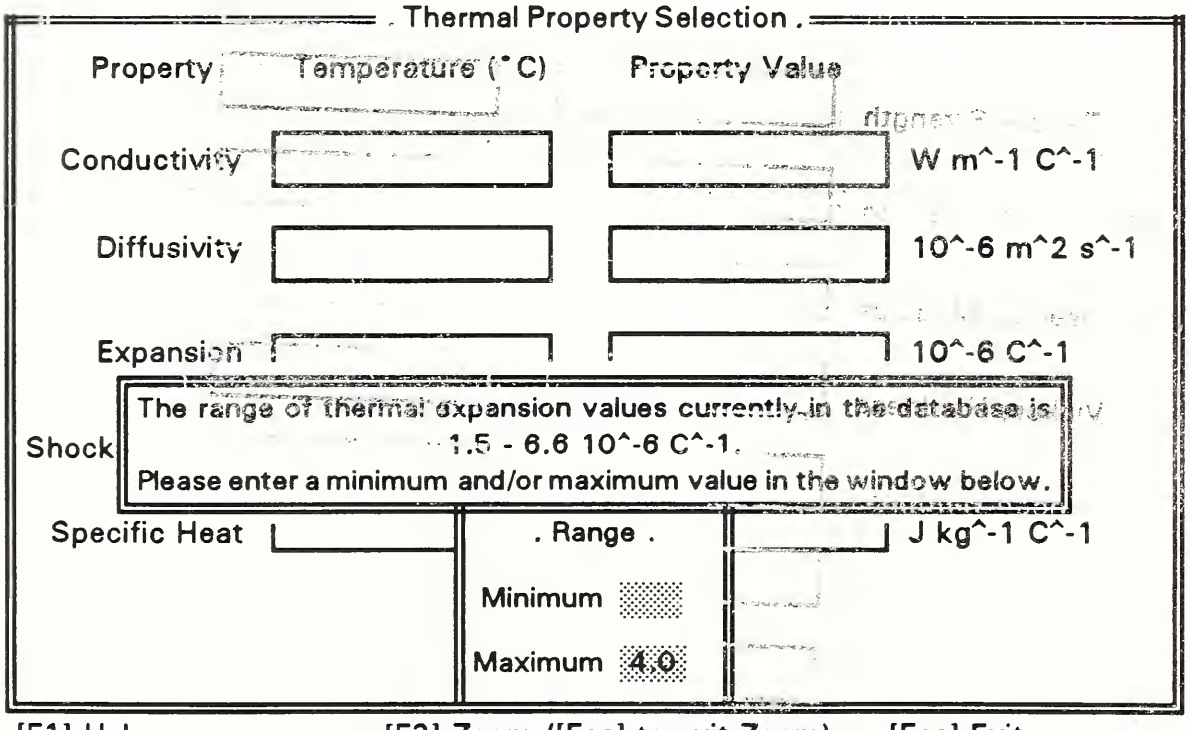
[F1] Help [F3] Zoom ([Esc] to exit Zoom) [Esc] Exit
[F2] Choices [F9] Ok, Continue Arrows move cursor

*The user positions the cursor on the Thermal Expansion Property Value prompt, presses F2, and a menu of choices appears.*



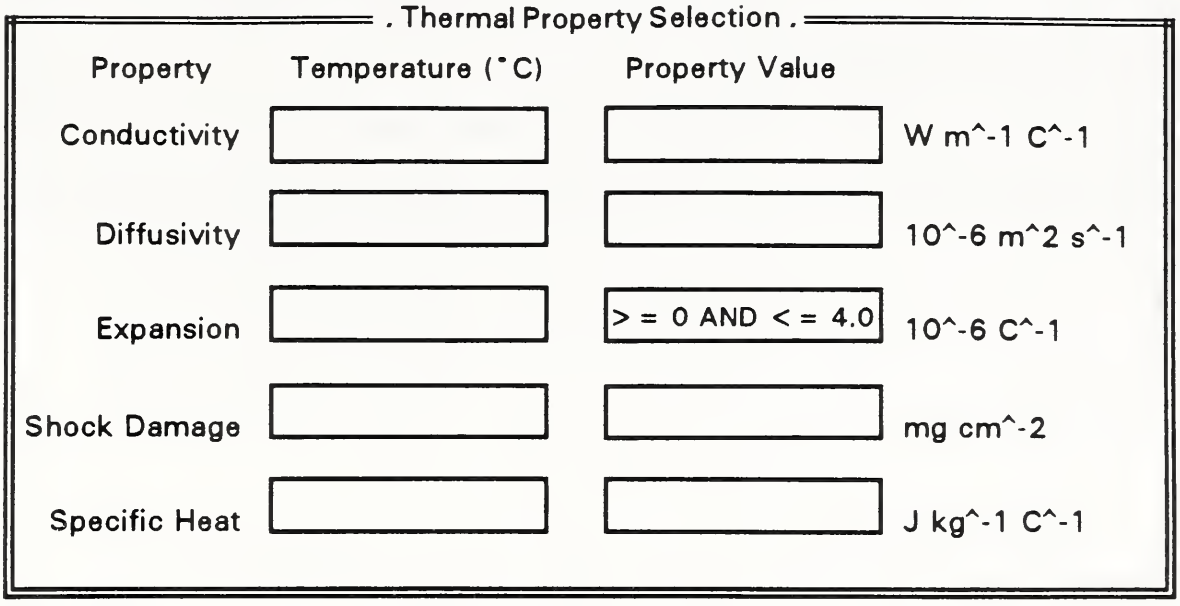

[F1] Help [F3] Zoom ([Esc] to exit Zoom) [Esc] Exit
[F2] Choices [F9] Ok, Continue Arrows move cursor

*The user chooses to specify a range and a message appears indicating the range of thermal expansion values in the database. A small window also appears into which the user may enter a minimum and/or a maximum value for the thermal expansion. The user types in 4.0 as a maximum.*

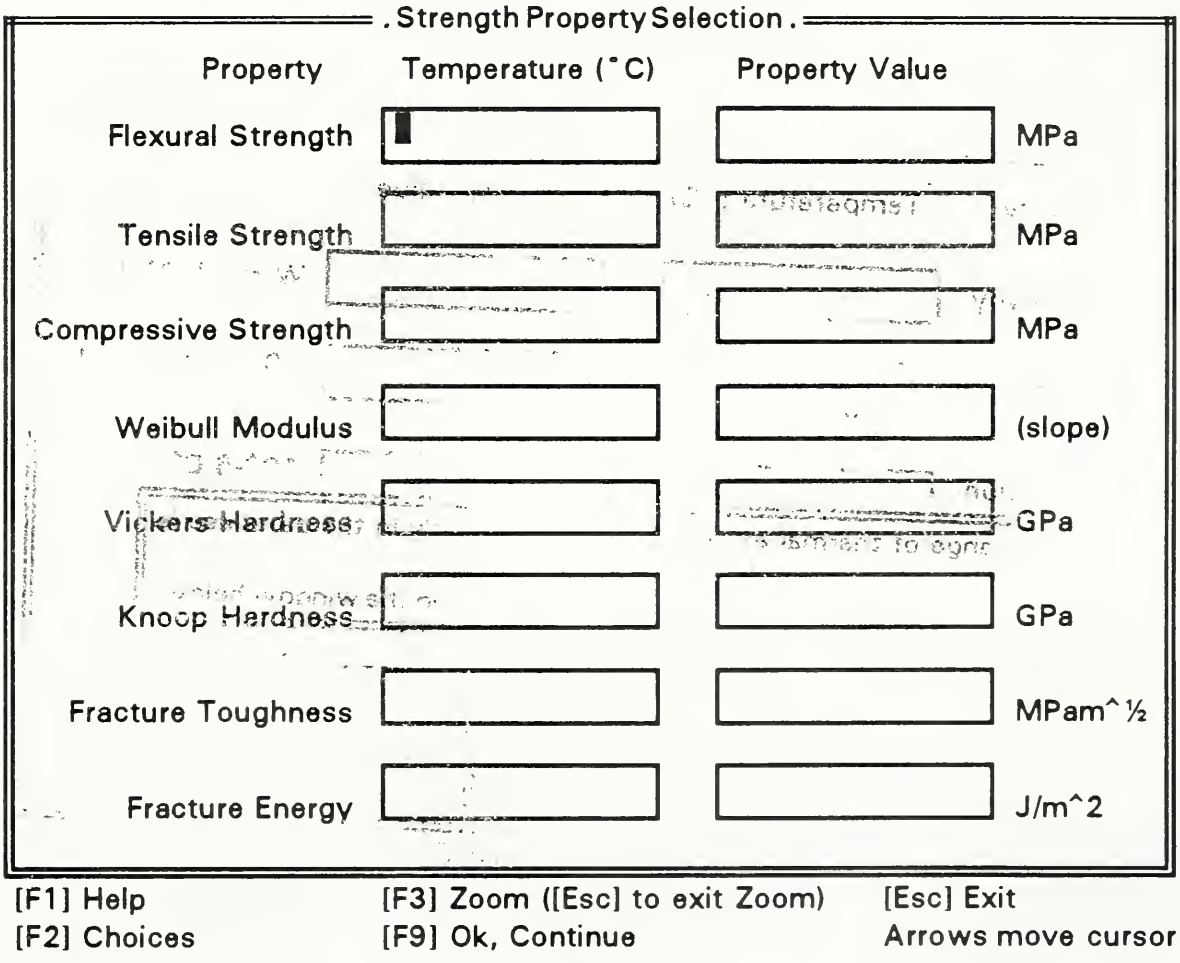



[F1] Help [F3] Zoom ([Esc] to exit Zoom) [Esc] Exit
[F2] Choices [F9] Ok, Continue Arrows move cursor

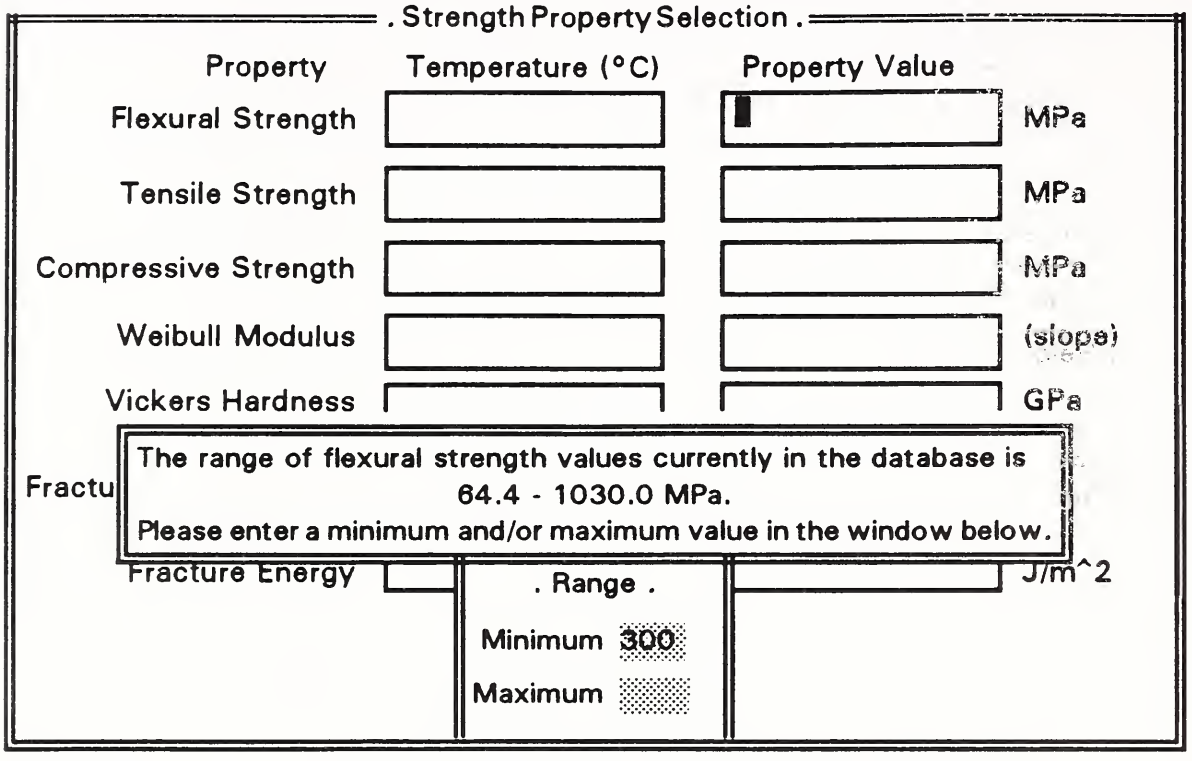
*The user then presses F9 to tell the system to accept 4.0 and transfer it to the Expansion Property Value prompt.*



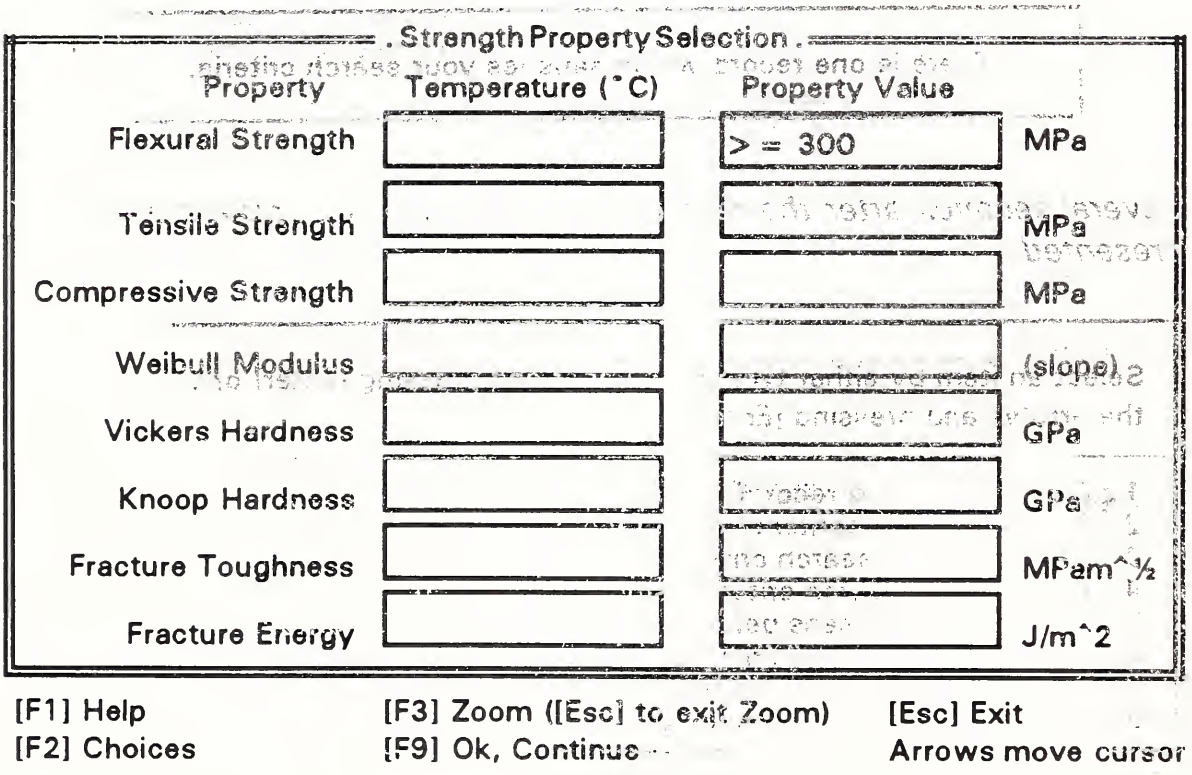

*Since all items of interest have been completed for this window, the user presses F9 to continue with the next step, which is to specify the desired flexural strength.*



*Following the same steps used for specifying thermal expansion, the user must place the cursor on the Flexural Strength Property Value prompt, press F2, and select "Range". Next, the user enters 300 for the minimum flexural strength value and the Strength Property Selection screen will then be displayed as below.*




*The user then presses F9 to tell the system to accept 300 and transfer it to the Flexural Strength Property Value prompt.*



*Satisfied with the entries on the screen, the user presses* **F9** *to continue with the next step, which is to perform the search. Once* **F9** *is pressed, a menu is displayed.*

Select an item by either typing a number and pressing [Enter] or using the arrows and pressing [Enter].

| | |
|---|---|
| 1 > | Perform search |
| 2 | Revise current search criteria |
| 3 | View a summary of the search criteria |
| 4 | Specify new search criteria using all query screens |
| 5 | Select query screens before specifying new search criteria |
| 6 | Reuse the search criteria from a previous query |
| 7 | Exit the Structural Ceramics Database |

[F1] Help [F9] Ok, Continue Arrows move cursor

*The user selects item 1 and the search begins. A message is displayed in the middle of the screen:*

Searching...
Please wait...

*Once the search has concluded, the system displays another message announcing the number of records found. In this case, the message appears:*

There is one record which satisfies your search criteria.

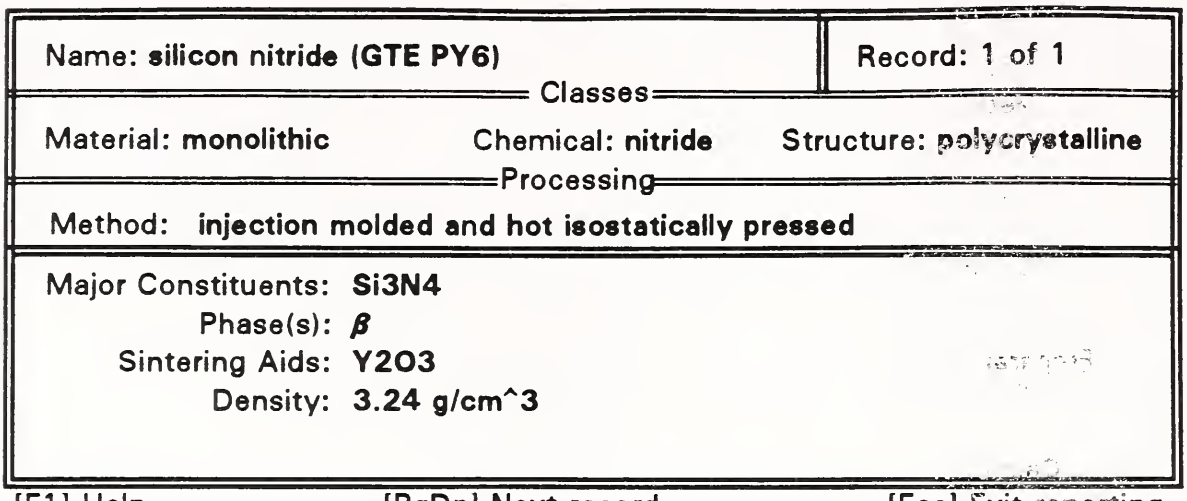
*Several seconds after the record count message is displayed a menu is presented.*

Select an item by either typing a number and pressing [Enter] or using the arrows and pressing [Enter].

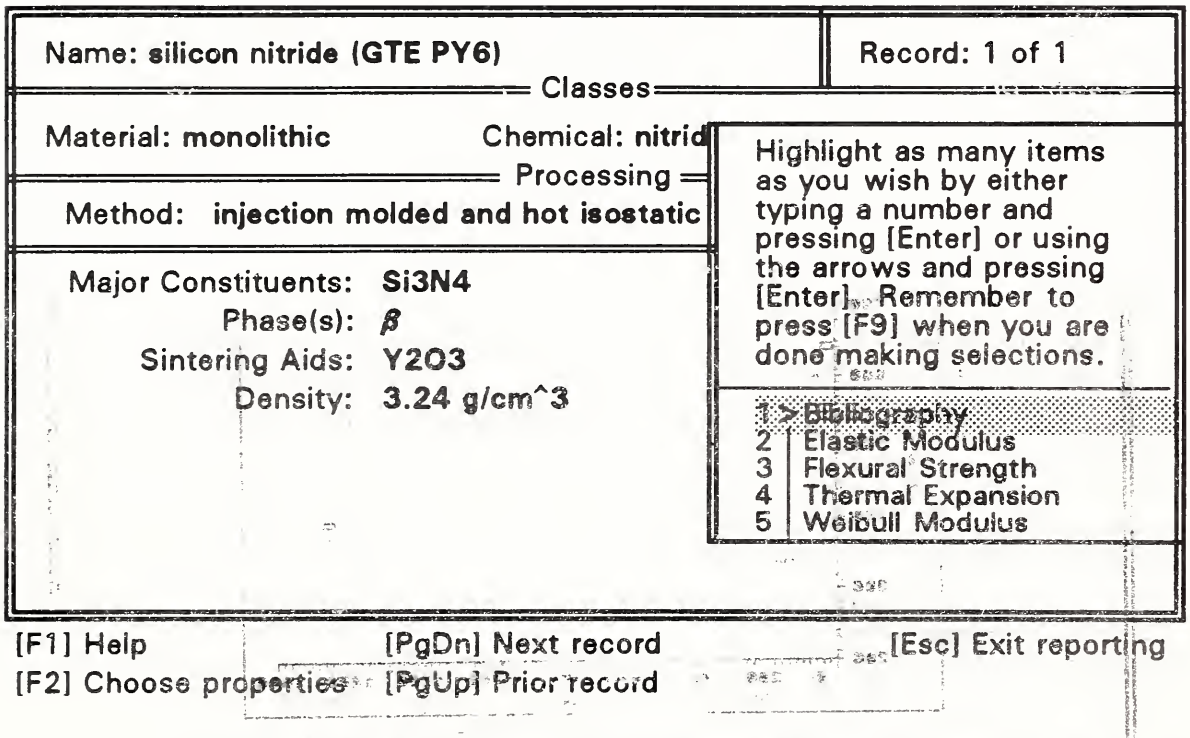
| | |
|---|---|
| 1 > | Display retrieved record(s) in a brief format |
| 2 | Display the full contents of all records |
| 3 | Revise current search criteria |
| 4 | Specify new search criteria using all query screens |
| 5 | Select query screens before specifying new search criteria |
| 6 | Save the current search criteria for future use |
| 7 | Reuse the search criteria from a previous query |
| 8 | Exit the Structural Ceramics Database |

[F1] Help [F9] Ok, Continue Arrows move cursor

*The user selects item 2 to display the full contents of all records and the record display begins with the material specification.*




*The user then presses* **F2** *to select property measurements for viewing. The material specification reporting screen will appear as below.*




*The user chooses Flexural Strength and Thermal Expansion from the menu by moving the highlight bar and pressing* **ENTER** *for each in turn. The user presses* **F9** *after making the selections. Thereupon the first property measurements screen for flexural strength is automatically displayed.*

| Name: **silicon nitride (GTE PY6)** | | Record: 1 of 1 |
|---|---|---|
| Flexural Strength | | |
| Temperature °C | Flexural Strength MPa | Crosshead Speed cm |
| 25 | 641 | .0064 |
| 1450 | 393 | .0064 |

Method: four-point bend

Notes: Instron Universal Testing Machine, Model 1123. Measurements at 1300°C and 1450°C used an ATS #3320 high temperature furnace. For room temperature tests, the bend fixture was made of steel. For tests at 1300°C and 1450°C, the bend fixture was made of SiC. The four-point bend fixture had an outer span of 3.81 and an inner span of 1.90 cm.

Preparation: Rectangular test bars, 51 x 6.4 x 3.2 mm. The tensile surfaces were ground, and the long edges of the tensile surface were chamfered.

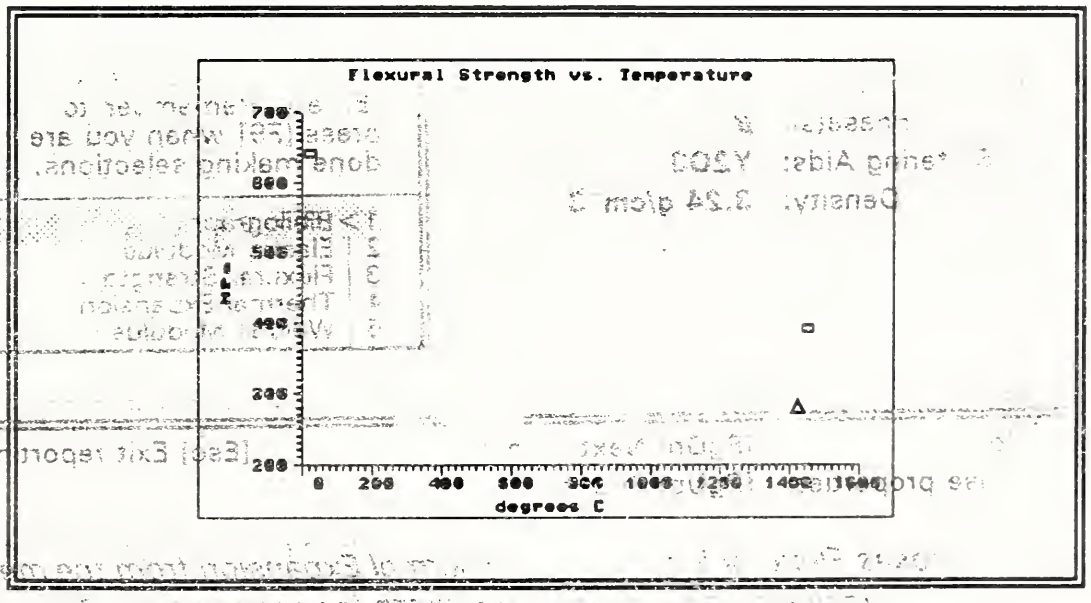
Cautions: Standard deviations were approximately 69 MPa. Specimens failed at tensile surface, edge, and subsurface flaws.

Environment: air

**Use arrow keys to pan the display since more information may be available.**

[F1] Help [PgDn] Next property [F8] Display graph
[F2] Choose properties [PgUp] Prior property [Home] Return to description

*The user presses F8 to display a graph of the data for this property.*



*The user presses* **ESC** *to return to the tabular display and then* **PGDN** *to view the next set of property measurements for thermal expansion.*

| Name: **silicon nitride (GTE PY6)** | Record: 1 of 1 |
|---|---|

Thermal Expansion

| Temperature °C | Thermal Expansion 10^-6 C^-1 |
|---|---|
| 1450 | 3.4 |

Method: dilatometer

Notes: Measurements were made on four specimens, from 25 °C to 1450 °C, using a Theta Industries Dilatronic II, Model 6024, apparatus.

Cautions: Measured on interval from 25 °C to 1450 °C.

**Use arrow keys to pan the display since more information may be available.**

[F1] Help [PgDn] Next property [Esc] Exit reporting
[F2] Choose properties [PgUp] Prior property [Home] Return to description

*The user then decides to exit reporting mode and presses* **ESC**. *A menu is displayed.*

Select an item by either typing a number and pressing [Enter] or using the arrows and pressing [Enter].

| | |
|---|---|
| 1 > | Display retrieved record(s) in a brief format |
| 2 | Display the full contents of all records |
| 3 | Revise current search criteria |
| 4 | Specify new search criteria using all query screens |
| 5 | Select query screens before specifying new search criteria |
| 6 | Save the current search criteria for future use |
| 7 | Reuse the search criteria from a previous query |
| 8 | Exit the Structural Ceramics Database |

[F1] Help [F9] Ok, Continue Arrows move cursor

*Finally, the user exits the database by selecting item 8 from the menu and the session ends.*

# Appendix B

## CONTACTS

If you have comments or questions about the database, Standard Reference Data would like to hear from you. Also, if you should have any problems with the diskettes or installation, please let us know by contacting:

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