Thermodynamic Database MALT for Windows with gem and CHD

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Abstract. We have revised the thermodynamic database MALT to match the window's environments and also to make it bilingual (English and Japanese). The main characteristic features are described with an emphasis on those functions which will be available in the new version. To facilitate the application of thermodynamic analysis on materials development and process analysis, the database MALT provides generalized programs for calculating chemical equilibria and constructing chemical potential diagrams. MALT encourages users to utilize thermodynamic data in the databases as well as their own in thermodynamic analysis on their own materials/processes problems. To facilitate it, MALT provides the function called "MALT Direct," which can make access to the data users prepare, and can utilize them in their own programs written in Pascal and compiled in Delphi. Some functions of the generalized calculation programs, gem and CHD, are also described in this report. © 2002 Published by Elsevier Science Ltd.

1. Introduction

The thermodynamic database MALT[1-3] (MAterials-oriented Little Thermodynamic database) was developed by a thermodynamic database task group, which was organized initially in the Japan Society for Calorimetry and Thermal Analysis and later became independent from the society. This task group started its activity with an aim at facilitating the utilization of the high-quality thermodynamic data in practical materials problems. In particular, its industrial use was highly encouraged. The present paper describes the main characteristic features of a new version of MALT together with related computer programs, *gem* [4] and *CHD*[5,6].

2. Objectives of Thermodynamic Database MALT

The main objective of constructing the thermodynamic database is to facilitate the utilization of the well-defined thermodynamic data in the industrial sectors. For this purpose, we made initial focuses on the inorganic compounds needed for understanding the chemical behavior of industrially important substances.

TABLE 1 Numbers of compounds stored in MALT and MALT2 in comparison with the numbers in the NBS tables(7). The state is given at 298 K.

Database	gas	gaseous ion	liquid	crystal	amorph ous	aqueous	total
MALT('87)	1438		53	1523	4		3018
MALT2('92)	2371		272	2284	5		4932
				(3324 state)			(5972 states)
NBS ('82)	1300	595	264	4668	36	(1032)	6863
							(7895 including aq)

Thus, collection was made on those chemical thermodynamic data (enthalpy change and Gibbs energy change for formation, and entropy at 298.15 K) and thermal data (heat capacities and enthalpy change for phase transition, if any) of inorganic compounds. Then it was extended to some organic compounds.

To ensure the thermochemical consistency among the stored data, the first reliance was placed on the NBS thermochemical tables published in 1982 [7]. For those compounds that are not given in the NBS table, particularly double oxides, the thermodynamic functions have been evaluated to be consistent with the NBS tables. Since value of the thermodynamic database increases with the number of stored compounds, efforts have been made to enlarge the number of compounds rather than to extend to the solution phases. In this sense, we keep the chemical thermodynamic standpoint.

When the chemical thermodynamic data are utilized among several compounds, the thermochemical network among these data is very important. For example, when one value for a particular compound is wrongly given, the evaluated thermodynamic properties associated with the system containing the wrongly given compound are always wrong. In other wards, when data are given correctly, addition of one compound gives rise to many benefits. In this sense, the mutual relation among the thermodynamic data is essential for the thermodynamic database. To maximize such benefits, the generalized programs for calculating the chemical equilibrium and for constructing the chemical potential diagram have been developed in parallel to the enlargement of the database. Particularly, the construction of chemical potential diagram for selected systems will be appropriate to judge the validity of the estimated or the evaluated new data. When the newly determined data cannot reproduce well-determined phase relations, we can judge that some thing wrong was taken place during the evaluation procedure. Such a procedure makes the quality of the thermodynamic database higher and more reliable.

On the other hand, it is impossible to provide the perfect thermodynamic database. Although the upgrade of the thermodynamic database is made from the long-term point of view, users in a particular field want to do some analyses in a very short period of time within available data or those data to be enlarged by their short-term efforts. This leads to the necessity for users to edit and create their own set of data. For this purpose, MALT provides functions of editing the thermodynamic data and utilizing the retrieved data in application programs. For example, immediately after changing the values in the thermodynamic functions, phase relations associated with thus revised values can be checked in the application programs, *gem* or *CHD*.

3. Main Characteristics of Database

3.1 Computer Language and Message language

Delphi was used to write the main parts of the database management system and the user interface of MALT. Related application programs for constructing chemical potential diagrams, *CHD*, and also for

calculating chemical equilibrium calculation with the Gibbs energy minimization technique, *gem*, were also written in Delphi. This makes it easy to make data transfer between the thermodynamic database MALT and the application programs, *CHD* and *gem*. As will be given below, the function of "MALT Direct" will be utilized from the users programs to be written in Delphi.

Message language is given in English or in Japanese. For a bilingual version, it can be switched between two languages.

3.2 Stored Thermodynamic Properties

TABLE 1 summarizes the number of the compounds stored in MALT published in 1987 and MALT2 published in 1992[3]. During the enlargement to MALT2, many double oxides of industrial importance and some organic compounds were added. Efforts will be made to enlarge the inorganic compounds and aqueous species. Appropriate estimation for heat capacity or entropy is therefore needed to improve coverage of the database.

3.3 Database Utilities

(1) Target databases

Since updating the main thermodynamic database cannot be made frequently in view of the current capability of the task group, it becomes essential to provide the facilities of handling those thermodynamic data, so that users can change the values or add new values. To facilitate this kind of user's activities, the thermodynamic database MALT/MALT2 allows users to handle their own data in users data file. To make it more user-friendly, users data in a user's ASCII file can be compiled to form a small database of users own. This user database can be targeted on retrieval of thermodynamic data. Although no direct editing is allowed on data stored in the main database, such data can be modified by users and stored in their own files and database.

(2) Retrieval

Retrieval is made in terms of (a) the chemical formula of compounds to be retrieved or (b) of the elements consisting the system to be considered. In the latter case, several modes are available. A typical one is to retrieve all compounds in a specified *n*-component system, which will be used in *gem* or *CHD*. Those compounds which contain specified elements will also be retrieved. For example, all silicates can be retrieved after selecting Si and O in this mode.

(3) Calculation facilities and related software

Facilities for preparing a thermodynamic table and a table for thermochemical properties associated with a chemical reaction are available as fundamental functions. Many options are provided to select the temperature range, temperature step, allowing or not extension beyond the temperature limit, etc. The numerical information in the thermochemical tables can be copied through clipboard to other software.

Advanced facilities for calculating complicated chemical equilibria are available, *gem* for calculating chemical equilibria [4] and *CHD* for constructing chemical potential diagrams [4]. *CHD* has been revised to provide more generalized diagrams as will be described later [5].
(4) MALT Direct

Interface with other software can be made through a special function of "MALT Direct." This is used to communicate with gem / CHD or with user's program written in Delphi. To illustrate how users can write the program in which retrieved data will be data-transferred from the thermodynamic database MALT, list of a sample program is given partly in Table 2. Here, MALTDirect() is the function of transferring the data from

the thermodynamic database MALT and creating an object in the type of TMALTCompoundsComponent. The following procedures are for obtaining the thermodynamic data as well as the information of compound name, valid temperature range and the stoichiometric numbers.

```
initialize(NCompound)
GetNameRangePhase()
GetThermoData()
```

4 Application programs

As generalized application programs, *CHD* and *gem* can be utilized by directly connected to the thermodynamic database.

4.1 Chemical equilibrium calculation, *gem*

Since *gem* is the Gibbs energy minimizer, the specification of calculations should be made before calculations. The calculation conditions can be input through a table sheet which is similar to sheet calculation software. The results are given in two sheets; one is about the molar base information, the other being the activity/fugacity information. Any parts of the sheets can be copied to other software through clipboard.

(1) Example I

Figure 1 shows typical results of the *gem* calculations. Here, all data in the result sheet given in mole were coped through clipboard to graph editing software where a graph was drawn in selected scales together with the text. The information given in the sheet for calculation conditions can be saved so that the calculation can be restarted using the same data under the same calculation conditions.
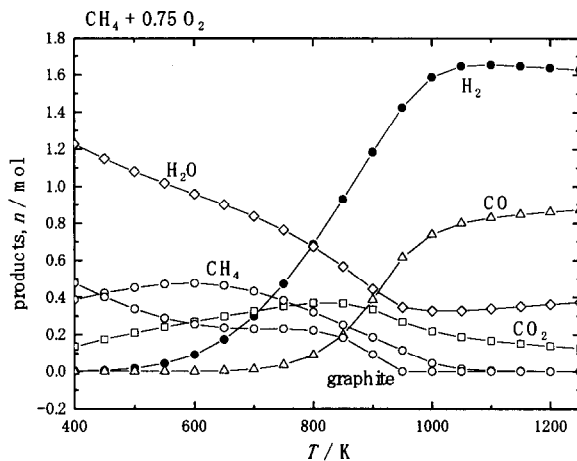

Fig. 1 Typical results of a series of chemical equilibrium calculations. The graphical plot was made in other graph editing software after the all information of the products was copied from gem. User can edit the graph in any software like this.
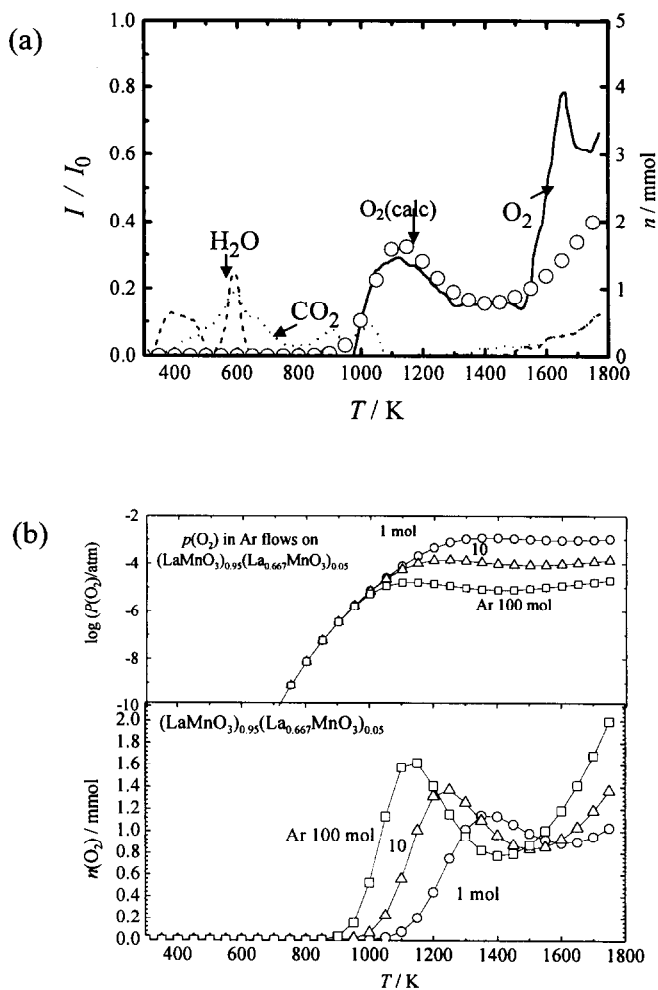
(2) Example II

Fig. 2 (a) Experimental results of the thermal analysis on the A-site deficient $(La,Sr)MnO_2$ perovskite oxide [8]. Open circles are the calculated oxygen evolution (Ar 100 mol). (b) Calculation results of gem for simulating oxygen evolution form the oxygen nonstoichiometric $LaMnO_3$ [9] in the thermal analysis by assuming the mass transfer due to the removal of the equilibrated gases.

Another example of applications of *gem* is about simulation for the thermal process which takes place within a thermal analyser. Usually, thermal analysis is made by increasing temperature in a selected heating

rate under a flow of selected gas in a given flow rate. The main purpose of doing thermal analysis is to obtain the kinetic information of various chemical reactions. In Fig. 2, typical results are given for the thermal analysis on A-site deficient and oxygen nonstoichiometric $LaMnO_3$ for which Thermogravimetric-Mass Spectroscopic (TG-MS) measurements were made to obtain the evolved gas amount as a function of temperature under an argon gas flow [8]. Since the measurement was made over a wide range of temperature so that we can expect that the results given in Fig. 2(a) are governed by the kinetic properties as well as the equilibrium properties.

To evaluate the equilibrium aspect of the experiment, we need the thermodynamic data which can reproduce the nonstoichiometric change of oxygen in perovskites oxide as functions of temperature and oxygen pressure. The thermodynamic representation of $LaMnO_3$-based perovskites was made in the ideal association model [9].

To extract the equilibrium aspect within the thermal analysis experiment, the following assumption can be made. Within a selected period of time, a selected amount of carrier gas was introduced into a sample chamber, and the equilibration took place between the given amount of gas and the sample substance, and then the equilibrated gas will be quitted out of the sample chamber. In a next step, another given amount of carrier gas will be introduced to obtain a next equilibrium at a stepwisely heated temperature. Specification of these conditions can be made in a sheet-type input method without difficulty. Here, kinetic factors are only considered for the flow of carrier gas. At each reaction period of times, equilibration is assumed to have been achieved.

Figure 2(b) shows the calculation results for selected argon flow rates. The upper part is the oxygen partial pressure within the sample chamber at respective steps. When the flow rate increases, the oxygen partial pressure decreases at high temperatures. This is because the increase in gas volume enhances the gas-evolving reaction and therefore reducing reactions are enhanced. The lower part indicates the amount of the evolving oxygen gas. Two-stage evolution of oxygen gas corresponds to the 'oxygen excess' and the 'oxygen deficient' ranges for oxygen stoichiometry in $LaMnO_3$ [9]. Since the higher flow rate enhances the reduction, the transient point from the 'oxygen excess' to the 'oxygen deficient' regions appeared at lower temperatures for the higher flow rates.

Even with such a simple assumption, the *gem* calculation results can reproduce the essential part of the TG-MS results. This implies many things for considerations on kinetics by means of thermal analysis. In this experiment, we can conclude that the surface reaction rate on the sample for gas evolution is faster than the equilibration time for evolved gas to become homogenous in a gas volume in the vicinity of the sample. Another important point related to the chemical equilibrium calculation is that the equilibrium features under a flow can be successfully simulated in a simple treatment for the calculation conditions of the Gibbs energy minimizer.

A similar analysis can be made for deposition of condensed substances when gaseous substances will be cooled in a similar process; an example is the dust formation from emitted gases out of electric furnaces. In this case, surface reaction rates are fast enough to achieve the equilibrium, whereas the equilibration is quite slow within the solid-solid reactions or diffusion in solids.

4.2 Construction of chemical potential diagram, *CHD*

The chemical potential diagram is a quite powerful tool for investigating the thermodynamic behavior of the materials stability and the materials compatibility. To maximize this power in materials science, the drastic improvements have been made in constructing algorithm; that is, the polyhedron method [5] is adopted to provide flexible treatments of phase relations in chemical potential spaces. This makes it possible to obtain the diagrams for multicomponent systems [6]. When the number of component increases, the complexity of phase relations increases significantly. This implies that when the phase relations in multicomponent systems will be treated, good manipulation methods are needed to inspect details of the phase relations. The computer program

CHD provides such methods to make full inspection on phase equilibria in the chemical potential space.

(1) Three component systems

In the new CHD program, generalization has been made for the way of selecting the coordinate axes; that is, not only chemical potentials but also inverse temperature or logarithmic pressure can be adopted. Particularly, adoption of inverse temperature as one of coordinate axes gives rise to some complicated features about how to select the appropriate coordinate axes. In Figs. 3 and 4, this is compared using the system where Si and C are included as parts of the systems. Figure 3 shows a typical example of the Ti-Si-C system at 1000 K, whereas Fig. 4 shows new types of the diagrams which indicates phase relations in the Si-C system as a function of inverse temperature.

In Fig. 3, the phase relations in the sub-binary Si-C system appear as the edges of a polygon; here, coordinates are given by the elemental chemical potential divided by *RT*. Phase relations associated with the ternary Si-Ti-C system are displayed inside the polygon for the Si-C system. Except for the representation of the compounds in the Si-C system as lines instead of polygons, Fig. 3 provides a reasonable display of phase relations in the ternary system on the two-dimensional diagram.

Figure 4 shows a case where projection on the two dimensional plane does not work well. In the three dimensional $\mu(\text{Si})/RT$- $\mu(\text{C})$ /*RT* -1/*T* diagram of the Si-C system, the stable areas of Si and C are represented by curved planes because their chemical potentials decrease with increasing temperature. When these phases are projected on a $\mu(\text{Si})/RT$- $\mu(\text{C})$ /*RT* plane, those areas are overlapped with that of SiC. In such a case, axes can be reselected to provide non-overlapped stable areas. For example, the logarithmic activity of Si and C are used instead of the elemental chemical potential in Fig. 3. Note that the elemental chemical potential changes with temperature, whereas the activities of Si, C remain constant in pure Si and C. In this case, the two dimensional log *a*(Si) vs. log *a*(C) plot is adopted to obtain a proper projection.

Another consideration can be derived from the above examination on phase relations in a system where

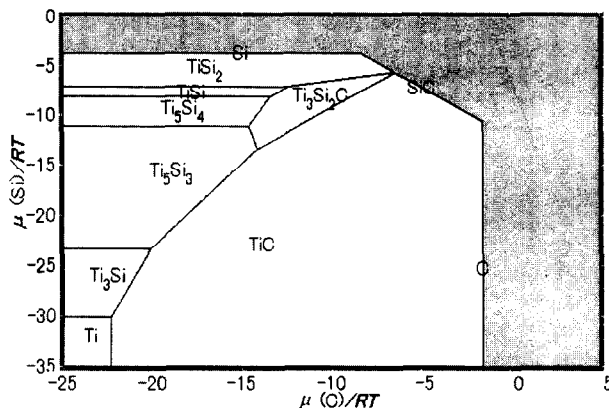The C – Si – Ti system at *P* =1.0 atm; *T* =1000.00 K

Fig. 3 The two-dimensional diagram for the Ti-Si-C system at 1000 K. The chemical potential of Ti is not used. Phase relations in the Si-C subsystem form a polygon, whereas phase relations belonging to the ternary system is displayed inside the polygon.

the inverse temperature is included as one of variables. That is, the fact that the elemental chemical potential decreases with increasing temperature is the important feature so that the projection in which this fact will be hindered is not appropriate for the thermodynamic analysis on the behavior of materials. In view of this, instead of the inappropriate two-dimensional diagram, the three-dimensional surface diagram should be used. In Fig. 4(a), the three dimensional surface diagram is plotted; here, all compounds are represented by a plane in a space. Thus, the qualitative feature of the chemical potential space including the inverse temperature can be easily gasped by taking a look at this type of diagram.

(2) Four component systems

For a four component system, a three dimensional diagram can be drawn by taking appropriate three coordinate variables out of four elemental chemical potentials. Here, the compounds are represented by polyhedrons instead of polygons in the two dimensional diagram. Again, care has to be taken in constructing a proper diagram. Figure 5 shows an example for the La-Ni-H-O system at 298.15 K. As diagram axes, μ(Ni), μ(H), and μ(O) are used and μ(La) is not used. In those compounds containing La, the chemical potentials of other elements (for example, μ(Ni)) are lower than those in Ni or NiO so that the compounds containing La cannot be seen from outside of polyhedrons consisting of 'polygons' of Ni, NiO, H_2O and H_2O_2. This is analogous to the feature in Fig. 3 that Ti containing compounds do not face to the open space but is covered by the 'segment line' compounds in the Si-C system.
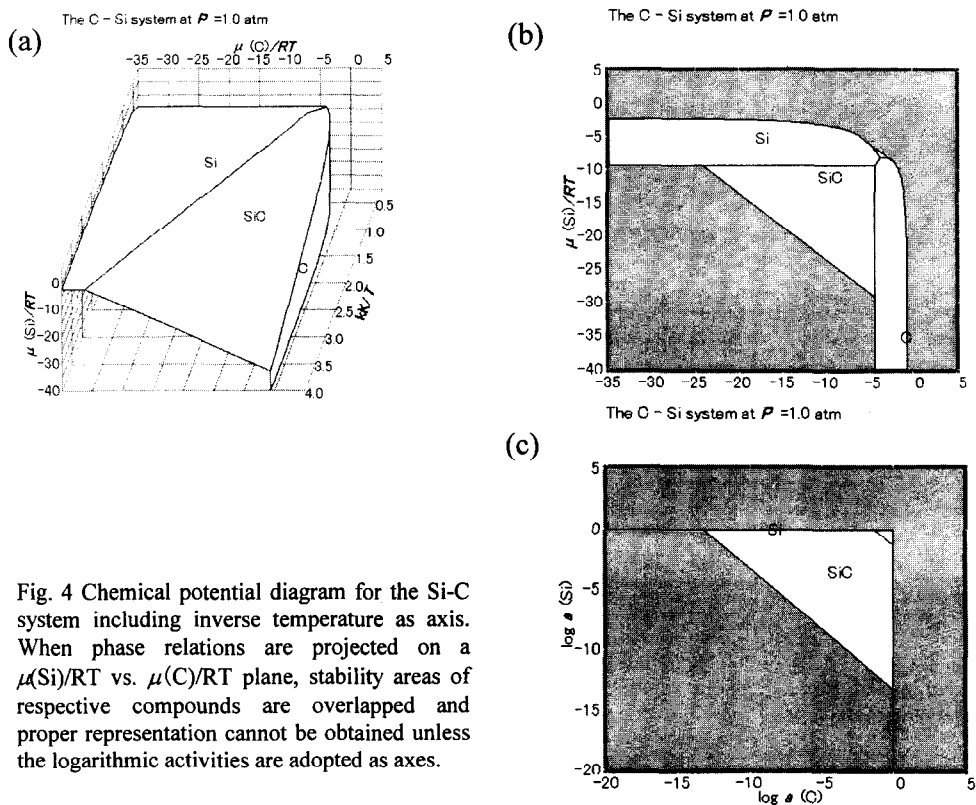

Fig. 4 Chemical potential diagram for the Si-C system including inverse temperature as axis. When phase relations are projected on a μ(Si)/RT vs. μ(C)/RT plane, stability areas of respective compounds are overlapped and proper representation cannot be obtained unless the logarithmic activities are adopted as axes.

In order to make phase relations visible in the three dimensional polyhedron-type diagram, some manipulation is needed. One way is to make selected stability areas transparent. This is shown in Fig. 5(b), where Ni and NiO are made transparent. In this plot, La_2O_3, $La(OH)_3$, $LaNi_5$, $LaNi_5H_{3.6}$, $LaNi_5H_{6.2}$ appear in the absence of Ni and NiO. Hydrogen adsorption and desorption takes place in the reducing atmosphere between $LaNi_5$ and $LaNi_5H_{6.2}$ through $LaNi_5H_{0.36}$. In the presence of water or oxygen, those alloys can be oxidized to form La_2O_3 or $La(OH)_3$. In Fig. 5(b), the oxygen potential is used as axis; in the oxidative atmosphere, the stability areas of La_2O_3 and $La(OH)_3$ actually appear. This suggests that $LaNi_5$ alloys seem to be covered with $La(OH)_3$. Even in such a phase combination of $LaNi_5/La(OH)_3$, the present diagram indicates the possibility of La_2O_3 formation at the $LaNi_5/La(OH)_3$ interfaces. These features seem quite interesting when comparison will be made with the performance of the $LaNi_5$ electrodes.

Another way of manipulating diagrams is to make a series of dissections by changing a fixed value for selected chemical potentials. Fig. 6(a) shows a $\mu(O)/RT$-$\mu(La)/RT$-$\mu(Ni)/RT$ plot for the same La-Ni-H-O system. Here the hydrogen chemical potential is hindered so that $La(OH)_3$ phase is not visible. Instead, $LaNi_5$, Ni, NiO and La_2O_3 are displayed in a visible manner. Although the hydrogen and related chemical potentials are not explicitly given in the figure, each point in the three dimensional diagram has a certain hydrogen chemical potential. This is because the original thermodynamic calculations were made in the four-dimensional chemical potential space and the results are just projected on the three dimensional diagram. In other wards, by fixing hydrogen partial pressure at a certain value, we can collect the points and construct a diagram. This can be called a dissection by fixing one chemical potential value. By fixing the hydrogen gas partial pressure at 10^{-30}, 10^{-10}, 10^{10} atm, a series of dissections can be setup as three dimensional surface diagrams as shown in Figs. 6(b), 6(c) and 6(d). When $p(H_2)=10^{-30}$ atm, phase relations among the La, Ni, O component does not change except for the appearance of $La(OH)_3$ phase at the borders with Ni and La_2O_3. When $p(H_2)=10^{-10}$ atm, La becomes to be hydrided, whereas $LaNi_5$ is not. Ni can be in equilibrium with $La(OH)_3$. When $p(H_2)=10^{10}$ atm, $LaNi_5$ is hydrided and also resulting $LaNi_5H_{6.2}$ can be in equilibrium with $La(OH)_3$. In other wards, under the hydrogen gas pressures below several atm, it will be hard for $LaNi_5H_{6.2}$ to coexist with $La(OH)_3$.

These diagrams provide some information on how the stability areas of respective compounds change with a parameter of hydrogen partial pressure. This kind of manipulation can be made in the interactive manner. That is, the value to be fixed can be changed manually under examination on how phase relations will change.
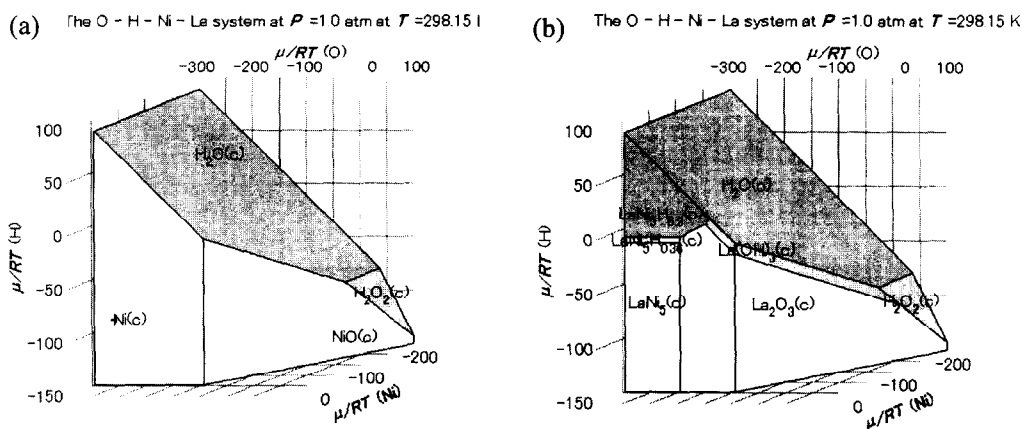

Fig. 5 Three dimensional chemical potential diagram for the La-Ni-H-O system at 298.15 K. (a) Since lanthanum chemical potential is not used, those compounds including La are not visible. (b) stability areas of Ni and NiO are made transparent so that other phases can be seen in the diagram.

(3) Touch mode

In many cases, the whole information of chemical potentials is required, if available, for a selected point in the displayed diagram. This can be made by touch mode, indicating the derived information on the chemical potentials of species and other thermodynamic properties given in a table. This can be copied to clipboard.

(4) Treatment for mixture phases

At present, mixture phases can, in principle, be treated in the construction of chemical potential diagrams except for those containing miscibility gap; for such mixtures, additional algorithm will be needed. At present, the ideal association model can be treated without problem.
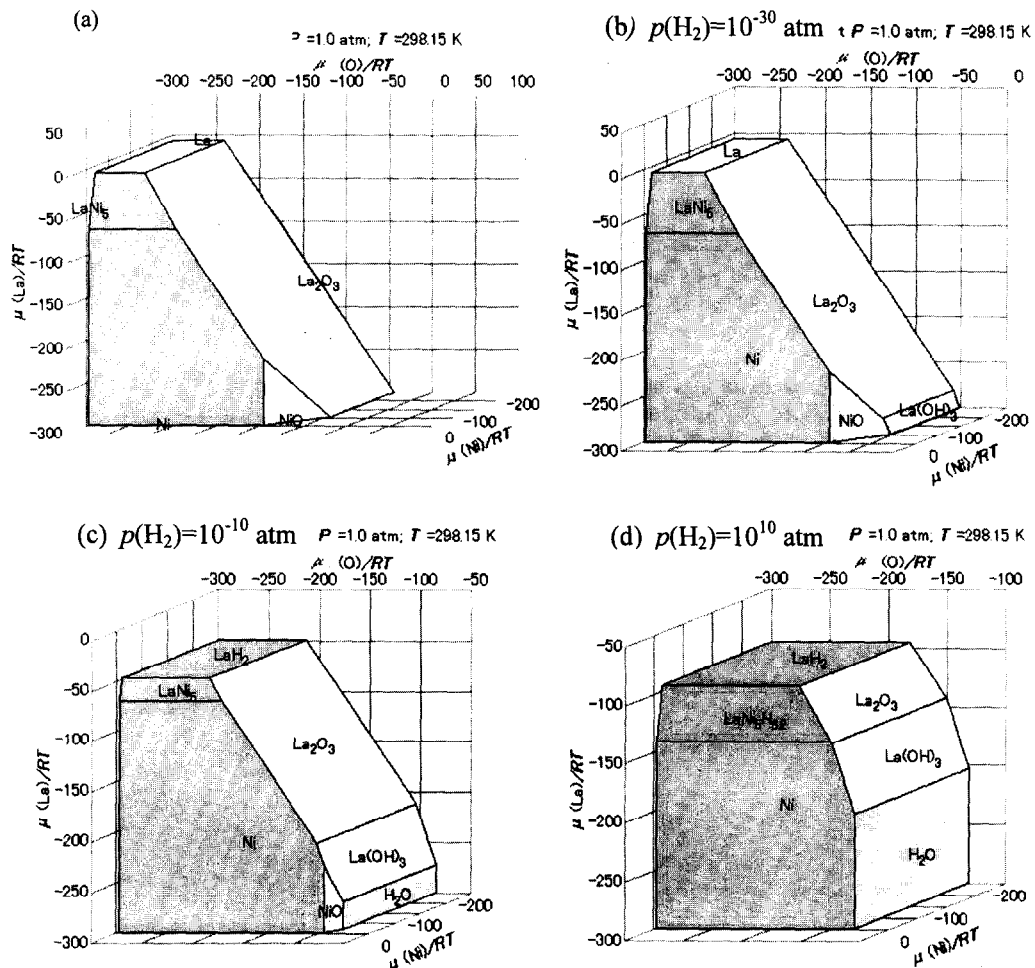
(5) Save diagrams

Fig. 6 a series of dissections of three dimensional diagram for the La-Ni-O-H system at 298.15. Partial pressure of hydrogen is selected at 10^{-30}, 10^{-10}, 10^{10} atm, respectively.

Saving the created diagrams can be made in various ways; Selection can be made among the Jpeg file, the bitmap file, or the window metafile. The window metafile is provided to allow users to edit further the diagram in other graph software, although this format is not popular. The diagram to be copied into clipboard is in the type of window metafile.

5. Dissemination

The first version MALT was published in 1987 and the second version MALT2 was published in 1992. As of May 2002, about 260 MALT2 systems have been sold through Kagaku Gijutsu-sha (Yushima 1-5-31, Bunkyo-ku, Tokyo 113, Japan, http://www.kagaku.com/malt). Since MALT2 is based on DOS, it can be run in any machines which provide DOS windows. Even so, the main message language of MALT2 is in Japanese, so that MALT2 is now used only inside Japan. Manual and some documents for explaining the database system and the related application programs are available in Japanese from Kagaku Gijutsu-sha. The demonstration version called mini-MALT is available through the above website. This consists of one exe file, mini database and other files which are needed to examine the functions of MALT. Since this mini-MALT is based on MALT2 so that message is given in Japanese alone. Although the mini database consists of a limited number of compounds, mini-MALT provides essentially the same functions of treating user data etc. This makes it possible for users to get idea what MALT can do and what MALT cannot. Particularly, MALT encourages users to write their own program to solve their own problems. To give examples how this can be done, samples programs are attached in the mini-MLAT. About MALT for windows, similar demo version, manual and related documents will be prepared in the near future and will be announced in the above website.

6. Conclusive Remarks

We have revised the thermodynamic database MALT to match the window's environments and also to make it bilingual (English and Japanese). The main characteristic features are described with an emphasis on those functions which will be available in the new version. To facilitate the application of thermodynamic analysis on materials development and process analysis, the database MALT provides generalized programs for calculating chemical equilibria and constructing chemical potential diagrams. To encourage users utilize thermodynamic data in the databases as well as their own, MALT provides the function called "MALT Direct," which can make access to the data users prepare, and can utilize them in their own programs written in Pascal and compiled in Delphi.

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9. H. Yokokawa, T. Horita, N. Sakai, M. Dokiya, *Solid State Ionics*, **86-88**(1996) 1161-1165.

Table 2. List of sample program to utilize the MALT retrieved data in user's program.

```
TForm 1 = class(TForm)
        procedure actMALTDirectExecute(Sender: TObject);
private
        FMALT : TMALTCompoundsComponent;
        FTemperature : Real ;
        Procedure ClearCells;
        procedure ShowStoichiometry;
        procedure ShowThermoDataAt(AValue: Real);

 end;
procedure TForm1.actMALTDirectExecute(Sender: TObject);
var Returncode:integer ;
    mode : integer ;
    ss : string ;
begin
    mode:=0;                                       {mode : 0 = retrieve without data structure.}
    FMALT.Free;                                    {Destroy the previously used data, if any.}
    FMALT:=MALTDirect(self, mode, Returncode);     {The Form(self) will be owner of the Datacomponent.}
    if FMALT<>nil then begin
        ClearCells;
        ShowCompounds;
        ShowStoichiometry;
    end else begin
        if        returncode=1 then ss:='MALT is not running.'
        else if returncode=2 then ss:='No retreived data available.  Retrieve compounds first.'
        else                        ss:='Error';
        StatusBar1.panels[0].text:=ss;
    End
end;


procedure TForm1.ShowCompounds;
var NCompound ,i :integer ;
    CompoundNameStr : string;
    TemperatureRangeStr : string ;
    PhaseStr : string ;
Begin
  if FMALT=nil then exit;
  with FMALT,StringGrid1 do begin
        initialize(NCompound);
        if NCompound<>0 then begin
           Rowcount:=NCompound+1;
           Cells[0,0]:='Name';
           Cells[1,0]:='Temp Range';
           Cells[2,0]:='phase';
           for i:=1 to NCompound do begin
               GetNameRangePhase(i,CompoundNameStr, TemperatureRangeStr, PhaseStr);
               Cells[0,i]:=CompoundNameStr;
               Cells[1,i]:=TemperatureRangeStr;
               Cells[2,i]:=PhaseStr;
           end;
        end;
  end;
end;

procedure TForm1.ShowThermoDataAt(AValue:Real);
var NCompound ,i :integer ;
    PhaseNo : integer ;
    ThermoDataStr:string ;
Begin
  if FMALT=nil then exit;
  with FMALT,StringGrid1 do begin
        initialize(NCompound);
        if NCompound<>0 then begin
           Cells[3,0]:='H(T)-H298';
           Cells[4,0]:='dHf(T)';
           Cells[5,0]:='Cp';
           Cells[6,0]:='S';
           Cells[7,0]:='dGf(T)';
           for i:=1 to NCompound do begin
               GetThermoData(i, AValue, PhaseNo, ThermoDataStr);
               Cells[3,i]:=GetNextStr(ThermoDataStr);
               Cells[4,i]:=GetNextStr(ThermoDataStr);
               Cells[5,i]:=GetNextStr(ThermoDataStr);
               Cells[6,i]:=GetNextStr(ThermoDataStr);
               Cells[7,i]:=GetNextStr(ThermoDataStr);
           end;
        end;
  end;
end
```