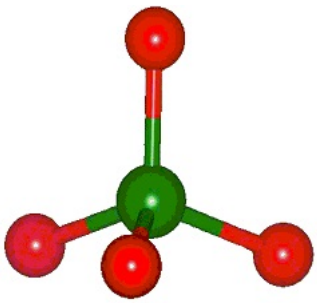
Miedema Calculator Users Manual



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1. Introduction

1.1 Overview of Miedema Calculator

Miedema Calculator is a thermodynamic software for predicting formation enthalpies of various alloys within framework of Miedema's Theory. Several user-friendly interfaces are designed for the following major functional modules, i.e. the formation enthalpies of binary intermetallic compounds based on the original Miedema's model and two more improved ones, the chemical, elastic and structural enthalpies of solid solutions, the formation enthalpies of amorphous alloys, the volume corrections upon alloying, and the formation enthalpies of ternary alloys based on various geometrical models.

Miedema Calculator is a user-interface program, which is designed and organized by Dr. R. F. Zhang et al. at Beihang University, for calculating the formation enthalpy (energy) of alloy based on the Miedema's theory and its derived models by Zhang et al. The name of the software comes from the name of the famous scientist Andries Miedema. In memory of his great contribution to the empirical thermodynamical model of "Cohesion in metals", we name this software as "Miedema Calculator".

1.2 Functionalities

1. Display and compare the model parameters of elements;
2. Perform the calculation of formation enthalpy of binary transition metal compound;
3. Perform the calculation of formation enthalpy of ternary transition metal compound based on various geometrical models;
4. Calculate the atomic size difference factor proposed by Zhang et al.
5. Calculate the Gamma parameter and the interfacial enthalpy of binary alloy system.
6. Calculate the chemical formation enthalpy, elastic mismatch enthalpy and structural formation enthalpy in a statistical solid solution.
7. Calculate the chemical formation enthalpy and topological formation enthalpy in

an amorphous alloy.

8. Calculate the volume change during alloying.
9. Periodic table of physical, thermodynamic and mechanical properties of elements.

Fig. 1.1 depicts the flowchart of the algorithm for the implementation of Miedema Calculator, which includes two general databases that store the basic elemental properties and model parameters, and five major functional modules: i) the formation enthalpies of binary intermetallic compounds; ii) the formation enthalpies of ternary intermetallic compounds; iii) the formation enthalpies of binary statistical solid solutions; iv) the formation enthalpies of binary amorphous alloys; v) the volume corrections of binary solid solutions and compounds upon alloying. A more detailed description for each module and an illustration is provided in latter sections.

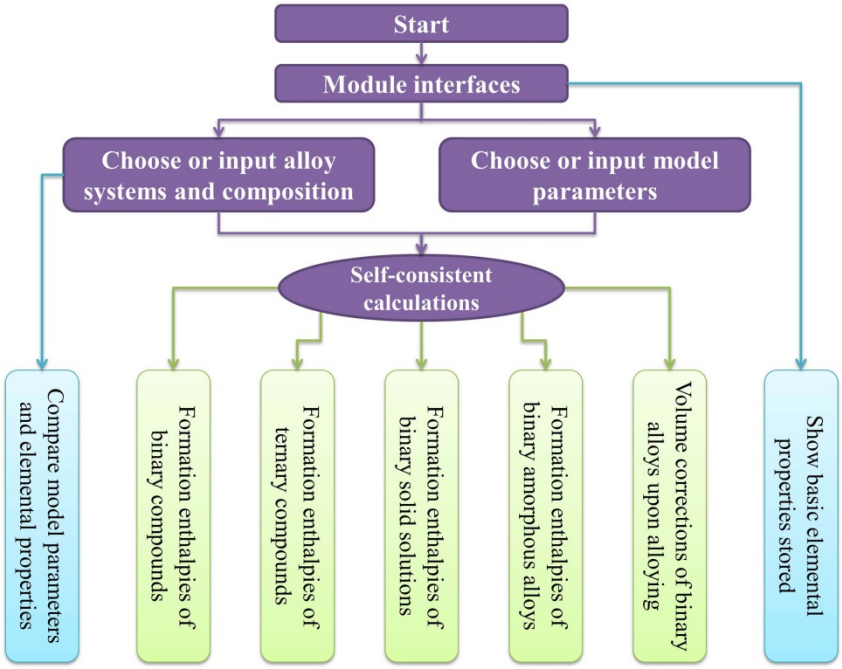

Fig. 1.1. Flowchart of the algorithm for the implementation of Miedema Calculator.

1.4 Restrictions

The calculation of formation enthalpy for intermetallic compounds implemented in Miedema Calculator is generally valid for binary/ternary transition metal alloy systems and alloy systems consisted of at least one transition metal. However, it can also be

applied for alloys with two/three non-transitional metals and polyvalence elements like N, B, C, etc, but it must be with caution in view of Miedema's suggestion that only if one knows that an alloy is truly metallic can one give a reasonably accurate estimation. For solid solutions and amorphous alloys, the application is restricted to the binary transition metal alloy systems, or some specific alloy systems consisted of at least one transition metal so far. We may refer to the original publications by Miedema et al. and Alonso et al. for more restrictions and guidance of applications of Miedema Calculator for solid solutions and amorphous alloys. In terms of ternary systems, all the geometrical models are implemented for intermetallic compounds, and other geometrical models may be included in the future.

1.5 Requirements

Miedema Calculator is written in C++ with dialog interfaces for different functional modules, and compiled and runs on Windows with the screen resolution 1024x768 or higher. It is contributed free of charge for non-commercial users.

1.6 Downloads

The latest software, additional information and tutorials of Miedema Calculator can be found on our website: https://sites.google.com/site/miedemacalc/ or http://miedemacalc.weebly.com.

2. Installation

The installation of Miedema Calculator is easy. In Windows, simply unzip the compressed file to a folder, e.g. D:/miedemacalc/, and then double click the executable file "MiedemaCalc.exe", one may get Miedema Calculator run with the first module interface showing up. One may get other module interface by choosing the list in "Menu->Module" submenu. To be noted that one need to send the registration form to miedemacalc@hotmail.com or register online at http://miedemacalc.weebly.com to get the password to decompress the encrypted file of Miedema Calculator.

3. Inputs and outputs

For each functional module, the minimum inputs are: i) the alloy system, ii) the alloy composition, and iii) model parameters for each element as presented in Fig. 1.1. The major outputs from self-consistent calculations are the formation enthalpies for modules i)-iv), and the volume corrections for module v). In addition, some critical model parameters and relevant intermediate results are also presented in module interface. To be noted that Miedema Calculator provides a special “input mode” by choosing the menu “Control”-> “Input mode” to make the model parameters editable in the region “Model parameters used”. In such mode, the self-consistent calculation is accordingly based on the model parameters that input/or is modified therein. It is suggested that the potential users read the brief tutorial in the next section.

4. Brief tutorial

We may suggest the new users to read the following tutorial. We now present only the five major functional module interfaces.

T.1. Standard formation enthalpy of binary intermetallic compounds

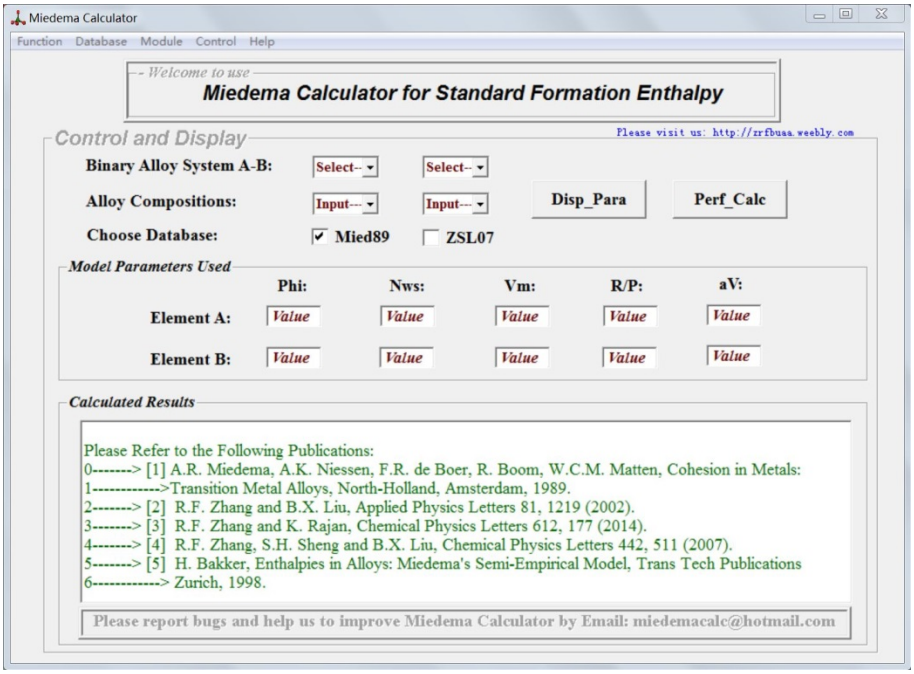

Fig. 4.1. The module interface for the standard formation enthalpies of binary intermetallic compounds.

Fig. 4.1 presents the module interface for standard formation enthalpy of binary intermetallic compounds. The original Miedema's model and two improved one are supported in this module. For the calculation of formation enthalpy of binary intermetallic compounds based on the original Miedema's model and two improved ones:

1) Launch the Miedema calculator by double click the software,
2) In menu, choose "Module"-> "Formation enthalpy of compound" to launch the module interface (see Fig. 4.1);
3) Choose the alloy system A-B from the drop list;
4) Choose or input the alloy composition;
5) Choose the database "Mied89" or "ZSL07", the default is "Mied89".
6) Click the "Disp_Para" button, you will get the model parameters shown in the region "Model parameters used";
7) Click the "Perf_Calc" button, it will perform self-consistent calculation for formation enthalpies, and the calculated results are shown in the region "Calculated Results".

T.2. Formation enthalpies of ternary intermetallic compounds

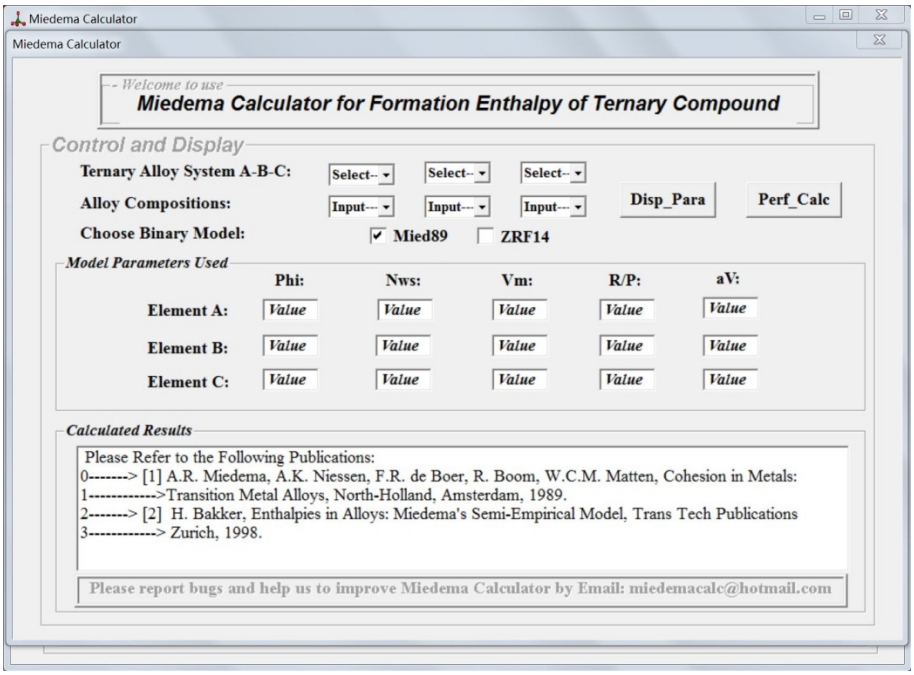

Fig. 4.2. The module interface for the formation enthalpies of ternary intermetallic compounds.

Fig. 4.2 presents the module interface for the formation enthalpies of ternary intermetallic compounds. The original Miedema's model and several geometrical models are supported in this module. For the calculation of formation enthalpies of ternary intermetallic compounds based on the different geometrical models:

1) Launch the Miedema calculator by double click the software;
2) In menu, choose "Module"-> "Formation enthalpy of ternary compound" to launch the module interface (see Fig. 4.2);
3) Choose the ternary alloy system A-B-C from the drop list;
4) Choose or input the alloy composition for each element;
5) Choose the binary model for the calculation of formation enthalpies of binary counterparts: "Mied89" or "ZRF14", the default is "Mied89".
6) Click the "Disp_Para" button, you will get the model parameters shown in the region "Model parameters used";
7) Click the "Perf_Calc" button, it will perform self-consistent calculation for formation enthalpies, and the calculated results are shown in the region

"Calculated Results".

T.3. Formation enthalpies of statistical solid solutions

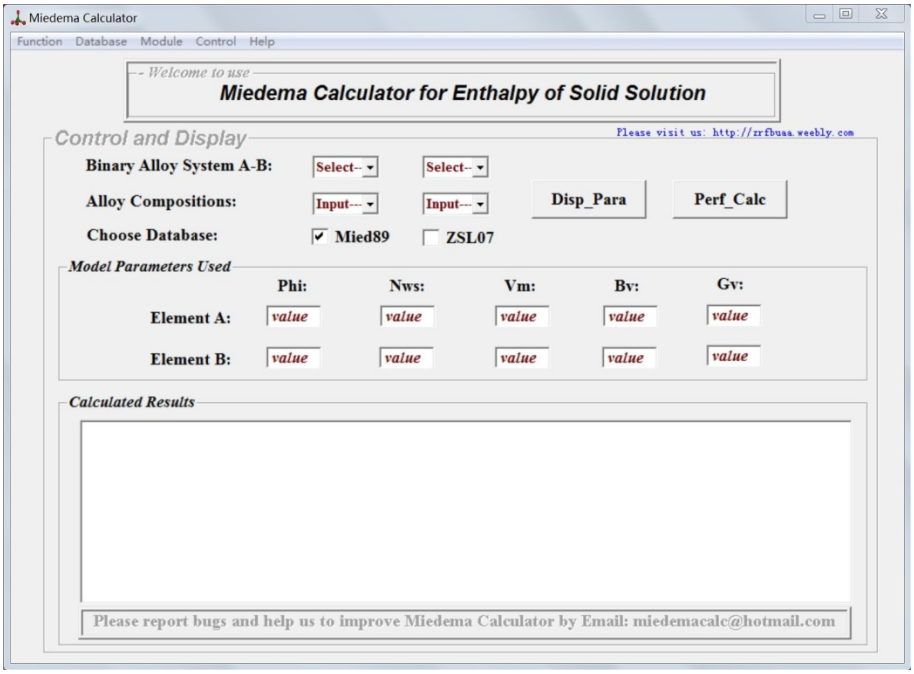

Fig. 4.3. The module interface for the formation enthalpies of statistical solid solutions.

Fig. 4.3 presents the module interface for the formation enthalpies of statistical solid solutions. The chemical enthalpies, elastic mismatch enthalpies and structural enthalpies based on Miedema's model and Alonso's model are supported in this module. For the calculation of formation enthalpies of binary concentrated solid solutions:

1) Launch the Miedema calculator by double click the software;
2) In menu, choose "Module"-> "Formation enthalpy of solid solution" to launch the module interface (see Fig. 4.3);
3) Choose the ternary alloy system A-B-C from the drop list;
4) Choose or input the alloy composition for each element;
5) Click the "Disp_Para" button, you will get the model parameters shown in the region "Model parameters used";
6) Click the "Perf_Calc" button, it will perform self-consistent calculation for formation enthalpies, and the calculated results are shown in the region "Calculated Results".

T.4. Formation enthalpies of binary amorphous alloys

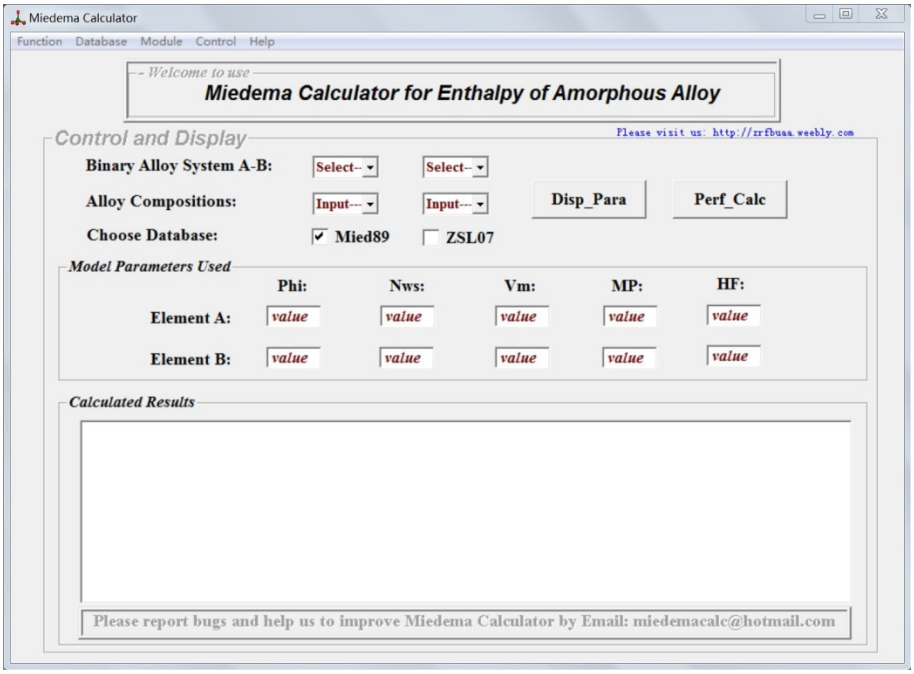

Fig. 4.4. The module interface for formation enthalpies of amorphous alloys.

For the calculation of formation enthalpies of binary amorphous alloys based on the Miedema's method and Alonso's method:

1) Launch the Miedema calculator by double click the software;
2) In menu, choose "Module"-> "Formation enthalpy of amorphous alloy" to launch the module interface (see Fig. 4.4);
3) Choose the binary alloy system A-B from the drop list;
4) Choose or input the alloy composition for each element;
5) Click the "Disp_Para" button, you will get the model parameters shown in the region "Model parameters used";
6) Click the "Perf_Calc" button, it will perform self-consistent calculation for formation enthalpies, and the calculated results are shown in the region "Calculated Results".

T.5. Volume corrections of solid solutions and compounds upon alloying

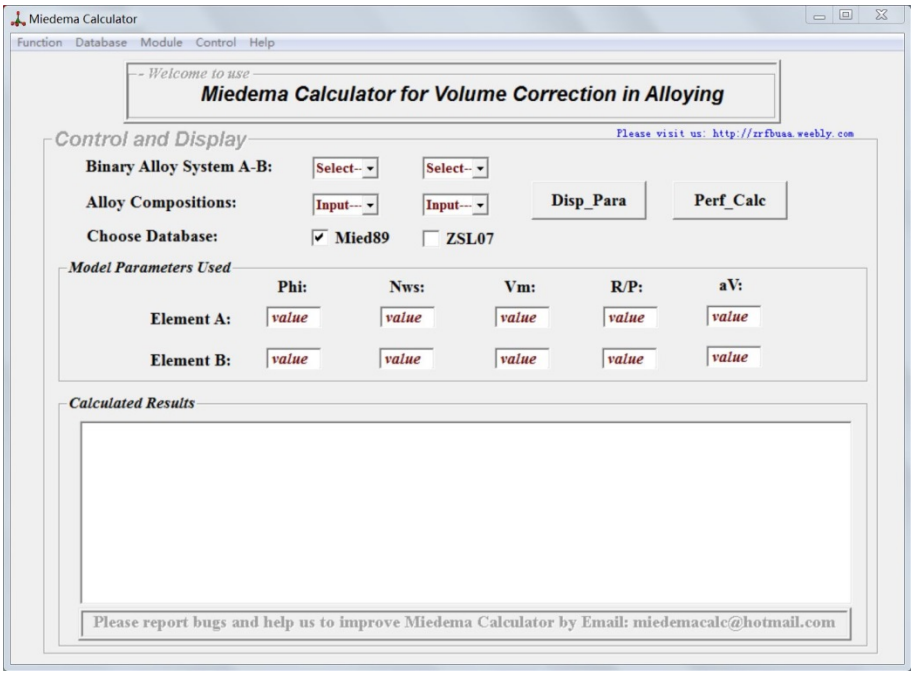

Fig. 4.5. The module interface for the volume corrections of solid solutions and compounds upon alloying.

For the calculation of the volume corrections of solid solutions and compounds upon alloying:

1) Launch the Miedema calculator by double click the software;
2) In menu, choose “Module” -> “Volume correction in alloying” to launch the module interface (see Fig. 4.5);
3) Choose the binary alloy system A-B from the drop list;
4) Choose or input the alloy composition for each element;
5) Click the “Disp_Para” button, you will get the model parameters shown in the region “Model parameters used”;
6) Click the “Perf_Calc” button, it will perform self-consistent calculation for formation enthalpies, and the calculated results are shown in the region “Calculated Results”.

T.6. Input mode

For the calculation of formation enthalpy of binary hybrids of transition metals (or other binary alloys) in “input mode”:

1) 1-6) is the same to the T.1. for the calculation of formation enthalpy of binary compounds;
7) In menu, choose “Control”-> “Input” mode to make the model parameters editable in the region “Model parameters used”;
8) Input or modify the values in the region “Model parameters used”;
9) Click the “Perf_Calc” button, it will perform self-consistent calculation based on new parameters, and the calculated results will be shown in the region “Calculated Results”.