

# MERLIN a versatile optimization environment applied to the design of metallic alloys and intermetallic compounds

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## Abstract

An important step in the design of alloys and intermetallic compounds using semi-empirical potentials is to determine the appropriate parameters, which best describe experimental and/or quantum mechanical *ab initio* results. This task is quite difficult as the data are not always consistent and complete and furthermore, they contain errors. To facilitate the modelling we use the optimization environment of MERLIN <http://merlin.cs.uoi.gr/>. This was applied to study a particular class of intermetallic compounds and alloys, which are very interesting, the so-called super-alloys, such as Ni–Al. We have fitted the properties of such intermetallic alloys and compounds utilizing a semi-empirical tight-binding potential in the second moment approximation. The potentials, which were produced in this way, were tested for properties at various temperatures, including segregation to surfaces and interfaces, and also for dynamical properties like the phonon density of states and mean-square displacements. We find a very good agreement to known experimental results and also a wealth of interesting information has revealed. Therefore the produced interatomic potentials present a realistic way to test scenarios which appear in the materials design.

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## 1. Introduction

Modern *ab initio* quantum mechanical computational methods have produced many important results, a great number of which are predictions, concerning the behavior of materials [1]. As the computational power increases, the set of systems, properties and situations that can be treated

broadens. On the other hand, even nowadays some problems are outside the reach of such exact methods and call for approximate treatment. Some important problems which need approximate treatment, are the thermodynamic properties of metallic alloys at surfaces and interfaces, a key problem in materials design [2]. When coping with such problems it is customary to invoke some approximation to the potential function of the system and determine the unknown parameters by minimizing an appropriate error function. A class of semi-empirical potentials which proved very useful for metallic systems includes the embedded-atom

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method (EAM) [3], Finnis–Sinclair potentials [4] and the tight-binding in the second moment approximation (TB-SMA) [5–7]. The error function has the form of a weighted norm, where each component is the difference between known experimental and/or ab initio zero temperature properties and the properties obtained using the approximate potential function [8,9]. The optimization problem can be stated as following: for a particular semi-empirical form find the parameters which best describe the intermetallic system. This problem is demanding because not all the data which are available for the fitting are equally relevant to the problem, and furthermore the data do not have the same accuracy. To help solve this problem one needs a flexible, transparent, easily implemented and controlled code. Those criteria are met by the optimization environment MERLIN. This environment includes many optimization methods in an homogeneous setup, menu driven control, scripting language, mechanism to store results of different optimization cycles. In effects, it allows a combined use of different optimization methods, which is done transparently without resorting to the complexities of each one, constraint the range of the parameters, fix the value of a parameter and so on. In addition the MERLIN optimization environment [10], which features its own programming language, MCL [11], that allows the programmer to build a strategy to find the best set of parameters. So far this approach has been used on a number of metallic alloy systems with success. Augmenting the procedure with molecular dynamics methods we have obtained a variety of properties essential in materials design and processes like growth, including the linear expansion coefficient, mean square displacements, both in bulk and at surfaces, and dynamical properties, such as phonon spectra, and atomic diffusion [12–17]. On the other hand using the Monte-Carlo method, in addition to the previous, we can access ordering and disordering phenomena in bulk, interfaces and at surfaces and segregation phenomena at interfaces and surfaces [18–22]. The purpose of the present work is to demonstrate the utility of the MERLIN environment and to show results concerning the thermodynamics of metallic alloys and intermetallic compounds.

## 2. Method

### 2.1. The MERLIN optimization environment

Multidimensional minimization is a common procedure applied in many fields. A variety of problems in engineering, physics, chemistry, etc., are frequently reduced to minimizing a function of many variables.

Minimizing a multidimensional function faces a lot of difficulties. There is no single method that can tackle all problems in a satisfactory way. The presence of constraints, even of simple ones, promotes the difficulty further. MERLIN [10] is a multidimensional optimization package designed to handle the following category of optimization problems: *Find a local minimum of the function:*

$$f(\mathbf{x}), \mathbf{x} \in R^N, \mathbf{x} = [x_1, x_2, \dots, x_N]^T, \quad (1)$$

under the box constraints:

$$x_i \in [a_i, b_i] \quad \text{for } i = 1, 2, \dots, N. \quad (2)$$

Special merit is taken for problems where the objective function can be written as a sum of squares:

$$f(\mathbf{x}) = \sum_{i=1}^M f_i^2(\mathbf{x}). \quad (3)$$

Seven different minimization algorithms are implemented in MERLIN. In particular there are two direct methods (Simplex and Roll) that use no derivative information. These are appropriate for small problems or when the objective function is subject to noise or when derivatives cannot be calculated. From the conjugate gradient family of methods, three algorithms are chosen: the Fletcher–Reeves, the Polak–Ribiere and the generalized Polak–Ribiere, while from the quasi-Newton family the DFP method and several versions of the BFGS method are coded. For the special case when the objective function is a sum of squares, an efficient Levenberg–Marquardt method is included. All algorithms and their implementation are described in detail in Ref. [10].

Some of the above algorithms require evaluation of the gradient. Since it is not always straightforward to code it, MERLIN provides accurate and efficient numerical approximations to the first derivatives and the Hessian matrix.

MERLIN is designed for interactive use. A user can select among the aforementioned minimization algorithms and perform a number of auxiliary operations through a friendly command line interface. For example one may want to change (or even remove) the constraints at some point of the minimization process or temporarily fix one or more of the minimization parameters at a certain value.

It has been realized that in order to efficiently handle a wide spectrum of problems one needs to combine several minimization methods, thus creating a minimization strategy. For this purpose MERLIN features its own programming language. The Merlin Control Language (MCL) [11] is a high level language that aids the user in implementing intelligent minimization strategies. The MCL compiler takes as input a strategy (appropriately coded in MCL) and outputs instructions that drive the minimization process.

MERLIN and MCL are both coded in standard ANSI Fortran 77 in order to be portable. The users need only to supply the objective function as an appropriate Fortran subprogram, and optionally gradient and Hessian information.

Newer versions of the package are available at <http://merlin.cs.uoi.gr/>.

There are certain advantages in having an optimization-specific environment and language. Among other things, it allows the user to concentrate on the minimization process and the physical properties under study, rather than dealing with “technicalities”, such as combining source code subroutines, dealing with arguments, etc. In addition it gives the user a variety of options and flexibility in implementing its minimization strategy. As a result the overall development time is greatly reduced, and the risk for errors in the user-written code is reduced as well.

Not many details of the MERLIN/MCL environment are provided, since we want to show the advantages of the MERLIN/MCL environment, not the implementation details. The corresponding Refs. [10,11] provide a complete description.

Once more, we would like to state that beyond its powerful minimization algorithms and wealth of options, the MERLIN/MCL environment is designed to “make things easy” and aid the user in the minimization process.

## 2.2. Semi-empirical potential

According to the Born–Oppenheimer approximation for adiabatic changes, for the potential energy of the ensemble of the ions we need to consider only the ionic positions. Therefore the potential energy can be written as

$$V = V(R_1, R_2, R_3, \dots, R_N). \quad (4)$$

This potential energy for the motion of the nuclei can accurately be obtained using state-of-art quantum mechanical computational methods. At present these methods have limits regarding the size, time scales, and the complexity of the systems they can be applied to. One way to alleviate these restrictions is to approximate the system using reasonable approximations. Such approximations are also useful in multiscale calculations. Many different approximations have been suggested for metals, coming under various names, forming the so-called many body potentials [3–7]. These are approximations to the full quantum mechanical problem and contain parameters to be obtained by suitable procedures. In such an approximation the potential energy is written as

$$V(R_1, R_2, R_3, \dots, R_N) = \sum_i^N F_i(R_i; R_a, R_b, \dots, R_n), \quad (5)$$

where  $R_a, R_b, R_c, \dots, R_n$  are the position vectors of the neighboring atoms of atom  $R_i$ .

Depending on the specific form of  $F_i$  we have a particular approximation. The one which we use is the so-called tight-binding potential in the second moment approximation (TB-SMA) [5–7]. The explicit form is

$$F_i = \sum_{i_x=1}^{N_\alpha} \left( \sum_{\beta} \sum_{j_{\beta}=1, j_{\beta} \neq i_x}^{N_{\beta}} A_{\alpha\beta} \exp \left( -p_{\alpha\beta} \left[ \frac{r^{\alpha\beta}}{d_{\alpha\beta}} - 1 \right] \right) - \sqrt{\sum_{\beta} \sum_{j_{\beta}=1, j_{\beta} \neq i_x}^{N_{\beta}} \xi_{\alpha\beta}^2 \exp \left( -2q_{\alpha\beta} \left[ \frac{r^{\alpha\beta}}{d_{\alpha\beta}} - 1 \right] \right)} \right). \quad (6)$$

In the above equation  $\alpha$  or  $\beta$  denote species A or B of the compound,  $A, p, q, \xi$  are the potential

parameters of the respective interaction terms,  $d$  is the nearest neighbor distance of the respective material, and  $i_\alpha$  are the sites occupied by atoms of type  $\alpha$ . This is not a pair potential because of the second non-linear term.

The unknown parameters relate to the strength and the range of both the attractive and the repulsive term, which are related to the electronic degrees of freedom. In order to make conduct with the full quantum mechanical problem and/or the experimental results we determine these parameters using a set of properties.

### 2.3. Construction of the error function

The set of properties we choose the potential to satisfy, forms a vector. The weighted distance from the vector with the desired values of properties, taken from experimental and/or ab initio results, defines the error function to be minimized using the MERLIN optimization environment. Such an expression is the following:

$$f(\mathbf{x}) = \sum_1^m w_i (p_i - \tilde{p}_i)^2, \quad (7)$$

where  $p_i$  are the values of the properties to which the fitting will be done,  $\tilde{p}_i$  are the properties calculated using the potential and depend on the parameters  $x$  and  $w_i$  are the weights.

A point about the input values for the fitting is that not all of them have the same amount of accuracy and therefore the weights must be larger for those properties known to be more accurate. In the particular application for Cu–Au system we choose higher weights for the lattice parameter, cohesive energy, bulk modulus, and lower for the elastic constants. All the mentioned properties comprise the vector of properties. Since we intend to produce a consistent potential for the whole range of the stoichiometries of the metallic compound, the vector must include the corresponding properties of all the intermetallic compounds present in the phase diagram and the pure metals. The parameters can be determined by minimizing the error function. It must be noted that the error function cannot be minimized exactly since the input data contain errors and, furthermore, not all

of them are consistent. This fact is not a problem, as long as most of the properties have converged to some suitable extent. At the end, we obtain a single model to present all the properties. Although approximate this model is consistent and this is exactly the advantage of the method, namely, it does not depend on the error from a single property.

Different strategies were followed for the choice of the properties which were included in the error function for the systems Ni–Al and Ni–Pt, and for the Cu–Au system, which will be explained in the specific subsection.

We have evaluated interatomic potentials of Ni, Al, Pt and Ni–Al, Ni–Pt ordered alloys within the SMA-TB model. The procedure consists of fitting the total energy expression (5) of the TB-SMA method to the first principles total-energy curves as a function of the volume for these materials. The determination of the  $\alpha$ – $\alpha$  and  $\beta$ – $\beta$  potential parameters of Eq. (6) ( $\alpha, \beta$  are the species) have been obtained by fitting to both fcc and bcc respective energy curves of pure metals, while the cross-potential parameters  $\alpha$ – $\beta$  have been evaluated by simultaneous fitting to the ab initio energy curves of the three ordered intermetallic compounds. This method has the advantage of providing potentials of good quality for pure metals. The fits have been performed using MERLIN [10,11]. This approach is very useful, especially in cases where not enough available experimental data are available in order to adjust the TB-SMA parameters.

### 2.4. Molecular dynamics

Using the expression of Eq. (6) with the adjusted parameters, we performed classical MD simulations for the pure metals and the ordered alloys in the canonical ensemble NVT at finite temperatures. Systems were constructed of 4000 particles arranged on the appropriate lattice structure. For the integration of the equations of motion we used a time step of 5 fs and the Verlet algorithm. Thermodynamical averages were computed over 50 ps trajectories after equilibration of 10 ps. At each temperature, the value of the lattice constant was adjusted to a

value resulting in zero pressure to the system. The atomic mean-square displacements were deduced from the local density profiles in the direction normal to the atomic layers. Finally, the phonon DOS were obtained by Fourier transforming the velocity auto-correlation functions [9].

### 2.5. Monte-Carlo method

The Monte-Carlo method is widely used for statistical and quantum mechanical calculations for various problems. Studying the thermodynamics of intermetallic compounds and alloys requires additional consideration. First of all, these systems are multicomponent and require the calculation of the chemical potential. In addition, their design includes internal defects, surfaces, pressure, and stoichiometry modulation. To cope with all these complex problems, a systematic and transparent method based on the particular many-body interatomic potential needed to be developed. The main point of the method is to produce a simulation-box by repeating an appropriate unit cell, and then be able to manipulate the atoms in the box in order to introduce surfaces, internal surfaces, or stoichiometric modulations. To perform such a task a suite of routines was produced. A windows interface to the routines helps the user to develop the simulation cell in a transparent way.

The particular Monte-Carlo realization includes constant pressure, chemical potential, and number of atoms. Constant chemical potential is utilized with the help of computational alchemy, i.e. in each simulation step the identity of a given atom is considered for mutation under the Monte-Carlo rules. Additionally to the constant pressure, each atom is also moved from its position to simulate thermal motion. This motion also relaxes the strains, and increases the acceptance ratio for the mutation of species. Therefore, all the dynamical effects are included. As a result we can study the following properties: chemical potential as a function of stoichiometry and temperature, segregation phenomena at surfaces and interfaces, various order parameters, lattice parameters, strains, and more.

## 3. Results and discussion

### 3.1. Ni–Al system

In Table 1 we report the calculated lattice constants of Ni<sub>3</sub>Al and NiAl at 0 K within the TB-SMA scheme together with the corresponding experimental values at room temperature [17]. The agreement between computation and experiment is very good. In the same Table we give also the bulk moduli of these ordered alloys. The deviation between calculated and experimental values of the bulk moduli is about 30%. In addition, the linear thermal expansion coefficient near room temperature for NiAl and Ni<sub>3</sub>Al has been deduced to  $17.4 \times 10^{-6}$  and  $15.9 \times 10^{-6} \text{ K}^{-1}$  respectively, while the corresponding experimental data are  $10.8 \times 10^{-6}$  and  $11.8 \times 10^{-6} \text{ K}^{-1}$  [17]. Furthermore, the computed mean-square displacements of Al and Ni are in excellent agreement with the experimental values from neutron or X-ray scattering [17]. Finally, the phonon DOS of NiAl and Ni<sub>3</sub>Al at 300 K are described with satisfactory accuracy within the TB-SMA model (cutoff frequency, position of peaks and presence of the gap [17]). This approach appears to reproduce the measured data with better accuracy than the TB-SMA, in which the parameters are obtained by fitting to several experimental data [8].

### 3.2. Cu–Au system

The Cu–Au system is of particular interest as it displays order–disorder transitions below the melting point. Its study has a long history both experimentally and theoretically. From the theoretical point of view it was the first metallic system to be studied using the Ising model. Although many results were produced, the description was

Table 1  
Calculated and experimental lattice parameters,  $a$ , along with the bulk modulus,  $B$ , for Ni<sub>3</sub>Al and NiAl [17]

Compound	$a$ (Å)- calc.	$a$ (Å)- expt	$B$ (GPa)- calc.	$B$ (GPa)- expt
Ni <sub>3</sub> Al (L1 <sub>2</sub> )	3.526	3.567	232	177
NiAl (B <sub>2</sub> )	2.895	2.886	222	158

far from realistic, since only the chemical disorder could be taken into account. Recently, with the use of the many-body interatomic potentials, all degrees of freedom, both chemical and positional, could be taken into account, without the necessity of any by hand change of the interactions close to the interfaces, surfaces and defects. By applying the machinery of the chemical potential, it was possible to assess segregation phenomena at and near interfaces, surfaces, and defects, which is of uppermost importance in the design of metallic systems. Additionally, the free energy, and other thermodynamic properties could be calculated giving a standard description of the system. This, in turn, permits the comparison with approximate statistical methods and also the advent of simplified thermodynamical functions suitable for direct fit to key experimental results. In this part we will describe the results that have been obtained so far, by citing the appropriate references and, in addition, we will present some recent results.

In order to determine the error function we used the experimental lattice parameter, cohesive energy and elastic constants of  $\text{Cu}_3\text{Au}$ . This was necessary, because the order–disorder transition is a phenomenon very sensitive to the potential parameters, as it depends on differences. It turned out that the order–disorder transition temperature for the constant volume condition is equal to the experimental temperature, but if we move to constant pressure conditions, and allow the atoms to relax we find a lowering of about 25% of the transition temperature. On the other hand, some thermodynamic properties, as for example the expansion coefficient, change of volume as we cross the order–disorder transition, and some dynamical properties like the mean-square displacements agreed well with the experimental results, provided that we plotted the results as a function of  $T/T_c$  [18]. We used the same potential parameters for the  $\text{CuAu}$  [21] and  $\text{CuAu}_3$  intermetallic compounds. To our surprise the findings were in good accord with the known experimental results. If we consider these findings with the ones on  $\text{Ni–Al}$  and  $\text{Ni–Pt}$ , we can conclude that different strategies do not necessarily lead to different results and depending on the available data one can build an appropriate vector of properties.

In the design of alloy systems a very important aspect are the segregation phenomena at interfaces and surfaces. It is well known that the properties of stainless steel depend on segregation of, for example, Ni atoms to the surface. In a similar way brittleness and strength are related to the segregation of impurities to internal boundaries. Having these facts in mind we studied the segregation profile near the surface of  $\text{Cu}_3\text{Au}$  [20,22] and near interfaces [19]. We found that at surfaces Au atoms segregate to the surface and that the amount of the segregated atoms changes with temperature, as can be seen from Fig. 1. In Fig. 2 we present the stoichiometry profile for slabs with different surface orientations at a given temperature. We can observe the different percentages of segregated Au atoms to the surface. On the other hand at twist and tilted  $\Sigma$  boundaries no segregation of either constituent could be observed [19].

Disordering is an important effect as it affects the properties of the materials. The  $\text{Cu–Au}$  system is ideal to study such phenomena, as there are many experimental results and relates to the class of super-alloys. One question in concern is the effect of surfaces and interfaces on the disordering. We have found that these changes in the lattice continuity increase the disordering and can lead to complete disorder below the order–disorder transition temperature [20]. Although the long-range order is lost, short-range order is observed. Fur-

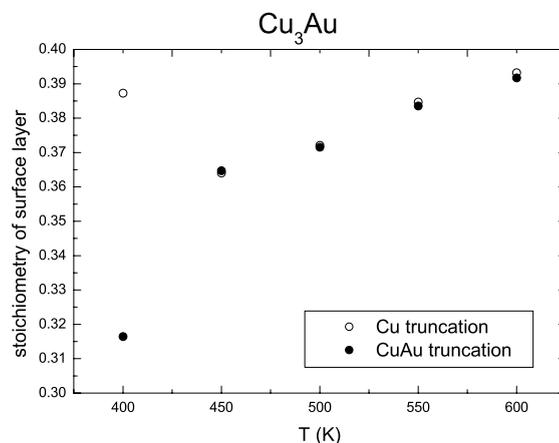


Fig. 1. Stoichiometry (atomic percent of Cu) at the (001) surface of  $\text{Cu}_3\text{Au}$  as a function of temperature.

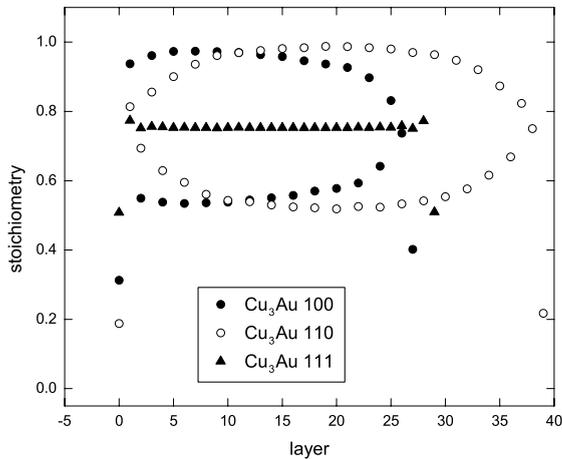


Fig. 2. Stoichiometry (atomic percent of Cu) profile of a crystal with the (001), (110) and (111) surface of  $\text{Cu}_3\text{Au}$ .  $T = 450$  K. The first and the last layer are the corresponding surface layers.

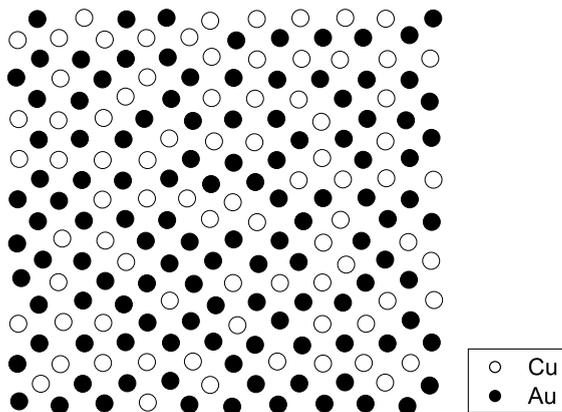


Fig. 3. Atomic configuration at the (001) surface of  $\text{Cu}_3\text{Au}$ .  $T = 450$  K.

thermore, Monte-Carlo simulations can produce the atomic arrangements at equilibrium, as can be seen in Fig. 3.

### 3.3. Ni–Pt system

Recently, the study of heteroepitaxial growth has been widely increased, due to its application in areas as catalysis, corrosion, magnetism, etc. In the following we will give an example of the application of our approach to the study of surface diffusion of Ni on Pt.

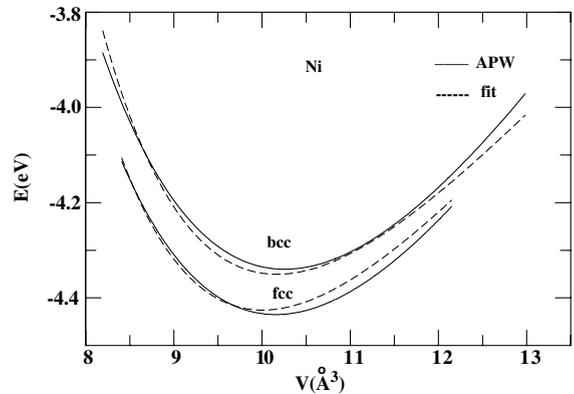


Fig. 4. Cohesive energies of Ni (with opposite sign) as a function of volume. Solid lines correspond to the APW results; dashed lines refer to the results of fit (Eq. (6)) using the MERLIN code.

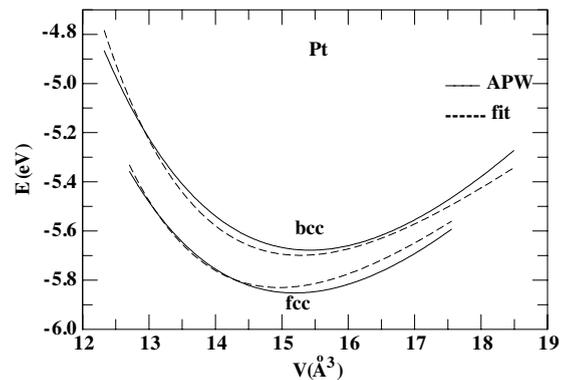


Fig. 5. Same as Fig. 4, but for Pt.

The interatomic potential for Ni and Pt has been obtained by fitting the cohesive energy of expression (6) to the volume dependence of the total-energy for both fcc and bcc structures, derived by first-principles APW calculations (Figs. 4 and 5 respectively). The cross-potential parameters for Ni–Pt have been evaluated by simultaneous fitting the ab initio energy curves of the three ordered intermetallic compounds (Fig. 6). The fits have been performed using MERLIN [10,11]. From this adjustment we find the lattice constants of metals and alloys at 0 K within the TB-SMA, which are presented in Table 2, together with available experimental values at room temperature [23,24]. The differences between computation and

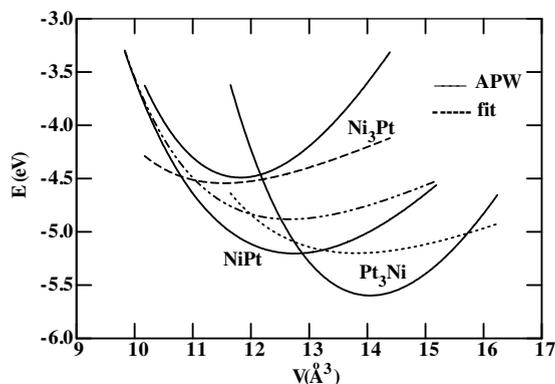


Fig. 6. Same as Fig. 4 but for the ordered alloys Ni<sub>3</sub>Pt, NiPt and Pt<sub>3</sub>Ni.

Table 2

Calculated and experimental lattice parameters,  $a$ , along with the bulk modulus,  $B$ , for Ni, Pt and their alloys

Compound	$a$ (Å)- calc.	$a$ (Å)- expt	$B$ (GPa)- calc.	$B$ (GPa)- expt
Ni	3.421	3.523	255	188
Ni <sub>3</sub> Pt (L1 <sub>2</sub> )	3.588	3.646	235	
NiPt (B <sub>2</sub> )	2.936		296	
Pt <sub>3</sub> Ni (L1 <sub>2</sub> )	3.810	3.837	283	
Pt	3.912	3.924	303	288

The experimental values of the lattice parameters for Ni, Pt are taken from Ref. [23] and from Ref. [24] for the alloys. The experimental data for the bulk modulus are taken from Ref. [25].

measurements are very small, except for Ni. In the same Table we report also the bulk moduli of metals and alloys together with available experimental data [25]. The agreement for Pt is better than for Ni. In addition, the thermal expansion coefficients near room temperature were obtained by MD simulations to be  $15.7 \times 10^{-6}$  and  $10.2 \times 10^{-6} \text{ K}^{-1}$ , for Ni and Pt, that compare well with the experimental values of  $12.5 \times 10^{-6}$  and  $8.9 \times 10^{-6} \text{ K}^{-1}$  respectively [23]. Furthermore, the phonon DOS of Pt at 90 K is well reproduced by the present model, showing a maximum frequency of 6.50 THz, in close agreement with the experimental value of 5.85 THz [26].

Using the above-mentioned interatomic potential in tandem with large-scale MD simulations in the temperature range of 300–1000 K, we have

studied the diffusion of single Ni adatom on Pt(111) and we have found that the diffusion coefficient shows an Arrhenius behavior with an associated migration energy of 230 meV and a pre-exponential factor of  $0.4 \times 10^{-3} \text{ cm}^2/\text{s}$ . Our value for the migration energy is higher than the reported value of 137 meV [27], obtained by static effective medium calculations. To our knowledge, there are no experimental data available for the diffusion of this system.

#### 4. Conclusions

The synergy of the optimization environment MERLIN, the MD and Monte-Carlo simulations and the TB-SMA of quantum mechanical origin has allowed to consider with success problems that are essential in the design and processes of metallic alloys. Good use is made of the available experimental and/or ab initio results to produce simple, realistic and coherent models which will allow fast and detailed examination of the possible scenarios that need to be tested in the process of materials' design. The systems may include surfaces, defects, impurities, multilayers and more complex structures. In addition the model can be used to bridge the different length and time scales.

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