Embedded atom method Potentials for Al–Pd–Mn Phases

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A novel embedded atom method (EAM) potential for the Ξ phases of Al-Pd-Mn has been determined with the force-matching method. Different combinations of analytic functions were tested for the pair and transfer part. The best results are obtained, if one allows for oscillations on two different length scales. These potentials stabilize structure models of the Ξ phases and describe their energy with high accuracy. Simulations at temperatures up to 1200 K show very good agreement with ab initio results with respect to stability and dynamics of the system.

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I. INTRODUCTION

The ternary intermetallic system Al–Pd–Mn has been of great interest in the last years, because it forms a high number of complex metallic alloy compounds (CMAs). In this paper we focus on the Ξ phases, which are approximated by the ternary intermetallic system Al–Pd–Mn. For ternary systems, like Al-Pd-Mn, establishing a functional relation between atoms is the embedded atom method (EAM). It implicitly includes many-body interactions by a term which depends on the environment of every atom. The potential energy of a system described with the EAM method can be written as

\[ E_{\text{pot}} = \frac{1}{2} \sum_{i \neq j} \Phi_{ij}(r_{ij}) + \sum_i F_i(n_i), \]  

with \[ n_i = \sum_{j \neq i} \rho_j(r_{ij}). \]

The first term in (1) represents the pair interactions between atoms \( i \) and \( j \) at a distance \( r_{ij} = |r_j - r_i| \). The function \( F_i(n_i) \) is the embedding energy of atom \( i \) in the host density \( n_i \). This density \( n_i \) is calculated as the sum over contributions from the neighboring atoms, with \( \rho_j \) being the transfer function of atom \( j \). It does not represent an actual physical density; \( n_i \) is a purely empirical quantity.

II. EAM POTENTIALS
For the pair and transfer part, we have tested three different combinations of analytic functions as model potentials. Potential I has oscillations in the pair potential but not in the transfer function. In contrast, potential II has oscillations only in the transfer function. Finally, a third potential has oscillations in both functions.

For the simple pair potential without oscillations we chose a Morse potential. It has a single minimum and is used in model II only:

$$
\Phi(r) = \Psi\left(\frac{r - r_c}{h}\right) D_e \left[\left(1 - e^{-a(r-r_c)^2}\right)^2 - 1\right].
$$

(3)

$\Psi$ is a cutoff function, where the free parameters $r_c$ and $h$ describe the cutoff radius and the smoothing of the potential. The remaining parameters are $D_e, a,$ and $r_e$; $D_e$ is the depth of the potential minimum, $r_e$ the equilibrium distance and $a$ the width of the potential minimum. The pair potential function with oscillations is adopted from Mihalković et al. 20:

$$
\Phi(r) = \Psi\left(\frac{r - r_c}{h}\right) \left[\frac{C_1}{r^{m_1}} + \frac{C_2}{r^{m_2}} \cos(kr + \varphi)\right].
$$

(4)

This “empirical oscillating pair potential” (EOPP) has been used in various works on complex metallic alloys and quasicrystals 11,13,14 as it provides great flexibility. The first term of (1) with the parameters $C_1$ and $\eta_1$ controls the short-range repulsion. The second term is responsible for the damping ($C_2, \eta_2$) of the oscillations with the frequency $k$.

The cutoff function $\Psi(x)$ is defined by

$$
\Psi(x) = \frac{x^4}{1 + x^4}
$$

(5)

for $x < 0$ and $\Psi(x) = 0$ for $x \geq 0$. This function guarantees that the potential functions as well as their derivatives up to the second order approach zero smoothly at the cutoff distance $r_c$.

Two different analytic forms were used as transfer functions; one allows for oscillations, the other one does not. The latter one is a simple exponential decay frequently used in established EAM potentials 5,13,15:

$$
\rho(r) = \alpha \exp(-\beta r),
$$

(6)

where $\alpha$ is the amplitude and $\beta$ is the decay constant. This function is used in model I. For models II and III, we used an oscillating transfer function, which is taken from Ref. 16:

$$
\rho(r) = \Psi\left(\frac{r - r_c}{h}\right) \frac{1 + a_1 \cos(\alpha r) + a_2 \sin(\alpha r)}{r^3}.
$$

(7)

The four free parameters are $a_1, a_2, \alpha$ and $\beta$, where $a_1$ and $a_2$ determine the amplitude of the oscillations, $\alpha$ is the wave vector and $\beta$ controls the decay.

The embedding function $F(n)$ was adopted from Ref. 14. It is based on the general equation of state from Rose et al. 17: The original form is given as

$$
F(n) = F_0 \left[\frac{q - p}{n} F_1 - \frac{p}{n} \right] - q + p \left[\frac{n}{n_c}\right]^q + F_1 n.
$$

(8)

The parameters in this function are $F_0, F_1, p, q$ and $n_c$. $p$ and $q$ are real values and $n_c$ is the equilibrium density. In this paper we use this function in the limit $p \to q$ and chose $n_e = 1$:

$$
F(n) = F_0 [1 - q \log n] n^q + F_1 n,
$$

(9)

because the original form is numerically unstable with our optimization algorithms.

The number of free parameters of our three potential models is comparatively large. The non-oscillating (oscillating) pair potential has 3 (6) parameters, and the non-oscillating (oscillating) transfer function requires 2 (4) values. All models share the embedding function with 3 free parameters. Every pair and transfer function has one additional parameter $h$ for the cutoff function $\Psi$. The cutoff radius $r_c$ is kept fixed at 7 Å. In a ternary system like Al–Pd–Mn with 12 potential functions, this adds up to a total number of 60, 48 and 66 parameters for the models I, II and III, respectively.

### III. FITTING PROCEDURE

All force-matching was performed with the POTFIT package of Brommer and Gähler 23, which has previously been used to optimize tabulated pair and EAM potentials. For this work, its capabilities were extended to analytic potential models.

All free parameters of the analytic functions were fitted to an ab initio reference database containing relaxed ($T = 0$) structures, snapshots from ab initio MD simulations at higher temperatures and a few strained samples (see Tables I and II). All ab initio calculations were performed with the Vienna Ab initio Simulation Package (VASP) 24, using the generalized gradient approximation (GGA) and the Projector Augmented Wave (PAW) method 25.

Two different optimization algorithms were used to fit the potentials. They both minimize the sum of squares defined by

$$
Z = \sum \omega_E |\Delta E|^2 + \sum |\Delta F|^2 + \sum \omega_S |\Delta S|^2,
$$

(10)

where $\Delta E$, $\Delta F$ and $\Delta S$ are the energy, force and stress residuals. These deviations are calculated as the difference of the ab initio and the EAM value, e.g.

$$
\Delta E = E_{\text{EAM}} - E_{\text{ab initio}}.
$$

$\omega_E$ and $\omega_S$ are global weights for the energies and stresses. $\omega_E = 22500$ was chosen to obtain potentials that yield very precise energies, but also reasonable forces. For configurations with about 150 atoms,
this effectively weighs the energies with a factor of approximately 50. The stress weight $\omega$ was set to 750, so that the total weight of the six stress tensor components per configuration is approximately equal to ten times the weight of all forces in one configuration.

The first optimization algorithm used is simulated annealing. It is based on the Metropolis criterion, where a decrease in the target function $Z$ is always accepted and an increase only with a probability $P = e^{-\Delta \mathcal{Z}/T}$. This allows the algorithm to escape local minima. The artificial temperature $T$ is steadily decreased during the optimization. To ensure that the fit converged to the global minimum, the optimization was restarted with a high temperature several times. Subsequently a conjugate gradient based method was applied to converge to the final optimum. During the fitting procedure, all parameters were confined to a predefined range by use of numerical punishments.

IV. REFERENCE DATA

The structures used as reference data are shown in Tables I and II. There are 119 configurations with a total of 16103 atoms. The number of reference datapoints is 49340. They consist of 48309 forces, 119 energies and 714 stresses.

| Al–Mn structures | Al–Pd structures |
|------------------|------------------|
| $\text{Al}_6\text{Mn}_4.\text{hP26}$ | $\text{AlPd}_3.\text{cP8}$ |
| $\text{Al}_3\text{Mn}_4.\text{aP15}$ | $\text{Al}_{12}\text{Pd}_3.\text{t116}$ |
| $\text{Al}_{12}\text{Mn}_4.\text{cI26}$ | $\text{Al}_3\text{Pd}_3.\text{hP5}$ |
| $\text{Al}_6\text{Mn}_4.\text{oC28}$ | $\text{Al}_3\text{Pd}_3.\text{tP4}$ |

TABLE I. Binary structures ($T = 0$) used to fit the potentials, with their corresponding Pearson symbol.

In addition to the binary and ternary structures, one reference configuration for each of the pure elements was also included. These were, in detail, $\text{Al}_6\text{cF4}$, $\text{Pd}_6\text{cF4}$ and $\text{Mn}_6\text{cF58}$. This was done to get reliable reference points for the calculation of the enthalpy of formation.

All atomic configurations from binary systems (Table I) were taken from the alloy database of Widom et al. and have been fully relaxed with ab initio methods. They were chosen to provide more data for the Pd–Pd and Mn–Mn interactions. Magnetism was not included in our ab initio calculation; it was shown that the manganese atoms in the $\Xi$-phases are nonmagnetic. Because the structures we want to investigate are on the aluminum-rich side of the phase diagram, there is only little data for the Mn–Pd interaction.

The reference configurations for the $\Xi$-phases are from different sources. The structures in Table II denoted with superscript a were taken from the alloy database. They were generated with the canonical cell tiling which creates hypothetical models by decorating a tiling with clusters. To compensate for the low amount of manganese in these samples and the hence resulting lack of data, five of the aluminum atoms were replaced by manganese in some configurations. Ab initio molecular dynamics simulations with VASP were run with these samples at 600, 1100 and 1800 K to obtain different local atomic configurations. These calculations were done in the generalized gradient approximation (GGA) with PAW potentials.

At the same time, ab initio structure optimization was carried out for two of the $\Xi$-phases. Particularly this were the $\Xi$-phase with the smallest unit cell, which contains about 152 atoms and is called $\Xi$ and the next bigger one, containing about 304 atoms, which is called $\Xi'$. All structures generated in the course of this optimization are denoted in Table II by superscript b.

To judge the stability of these structures, their energy is compared to a mixture of competing phases, the convex hull. This hull, defined over a ternary phase diagram, contains the cohesive energies of all stable compounds as vertices. If the energy of a structure is above this convex hull, it could decompose into the neighboring structures and thus lower its energy. If the energy of a new structure is below the convex hull, it is considered to be thermodynamically stable. The structures which define the convex hull for the $\Xi$-phases, are $\text{T-AlPdMn}$, $\text{Al}_2\text{Pd}_3\text{Mn}_3$, $\text{Al}_{12}\text{Pd}_3\text{Mn}_7$ and $\text{Al}_2\text{Pd}_3\text{Mn}_9$. They have also been included in the reference database. A detailed description of these phases and the convex hull is given in Ref.

V. RESULTS

We determined parameters for all three potential models from the reference data described above. The root mean square (RMS) errors for forces, energies and stresses after the optimization are in the same order of magnitude for all models (see Table II). While model III
has the smallest errors for forces and energies, model I has the biggest errors for all three quantities. Model II has the smallest stress deviations. While the force error for model I is about 20% larger than the one for model III, the energy error is significantly larger with about 50% difference.

| RMS errors for | Model I | Model II | Model III |
|----------------|---------|----------|-----------|
| forces         | 265.63  | 221.40   | 220.07    |
| energies       | 19.36   | 14.49    | 12.53     |
| stresses       | 99.99   | 76.83    | 98.30     |

TABLE III. Root mean square errors after the optimization for forces (in meV/Å), energies (in meV/atom) and stresses (in kPa). This data is calculated with the reference configurations used for fitting the potentials.

A graphical representation of these errors can be seen in Fig. 1. The scatterplots in the upper row display the energies of the reference data. Forces are shown in the lower row. The range of the force plots is due to the many high temperature MD simulations that are included in the reference data. The forces therein can become very large because of the short interatomic distances that may occur at these temperatures.

![Scatterplot for energies and forces with the EAM values on the vertical axis and the ab initio reference data on the horizontal axis. The insets are magnified by a factor 4.5.](image)

FIG. 1. Scatterplot for energies and forces with the EAM values on the vertical axis and the ab initio reference data on the horizontal axis. The insets are magnified by a factor 4.5.

These errors cannot solely be used to judge the quality and transferability of the potentials. For that purpose another set of ab initio data has been extracted from the structure optimization. It has not been included in the reference data and can be used to determine the transferability of the different potentials. The same errors as before have been calculated and can be seen in Table IV. As with the reference data, model III has the lowest force and energy errors. The relative error of the energy is about 0.2%, for stresses about 5% and 550% for forces. This is due to the fact that all configurations in this test data are ground state structures and therefore only contain very small forces.

| RMS errors for | Model I | Model II | Model III |
|----------------|---------|----------|-----------|
| forces         | 141.90  | 131.90   | 130.46    |
| energies       | 10.42   | 10.47    | 10.28     |
| stresses       | 32.39   | 23.76    | 36.89     |

TABLE IV. Root mean square errors for forces (in meV/Å), energies (in meV/atom) and stresses (in kPa). This data is calculated with test data, containing only structures that were not included in the optimization process.

The errors for the test data in Table IV are smaller than those of the reference configurations in Table III because there are only ground states included and no high temperature MD runs.

Based upon these simple energy and force considerations, all the potential models appear to be of similar quality. Model III, however, should be slightly superior to the other two potentials. Further tests are necessary to determine the performance of the potentials in different situations. They will be presented in Subsection VB.

### A. Structure Refinement

In Ref. 24 the structure of the Ξ-phases of Al–Pd–Mn has been optimized by energy minimization in ab initio and molecular dynamics simulations. We use several of the structures tested there to judge the quality of the optimized potentials. The Ξ-phases consist of columns of pseudo-Mackay icosahedral clusters (PMIs) 25 a slight deviation of the famous Mackay icosahedron.

Every PMI cluster consists of a single atom at the center with a first shell of an experimentally poorly determined number of aluminum atoms. The second shell is an icosahedron of 12 transition metal atoms and the outer shell an icosidodecahedron of 30 aluminum atoms, see Fig. 2. Almost all atoms of the Ξ-phases belong to these clusters. It is difficult to measure the exact number of atoms in the first shell because aluminum atoms are hard to observe in diffraction experiments.

For the lowest quasicrystal approximant, the ξ-phase, there are four PMI clusters in one unit cell. Several different occupancies of aluminum atoms in the first shell were tested in Ref. 24. Each configuration was denoted by a single number, giving the average number of aluminum atoms per cluster. Structures from eight up to eleven atoms per PMI were generated and tested.

The results with the different potential models can be seen in Table IV. All structures were completely relaxed with ab initio methods, the corresponding ab initio energy is given in column 2. The energies of these configurations with the generated EAM potentials have been calculated after subsequent relaxation with the respective potentials. This relaxation causes small displacements of the atoms from their ab initio determined positions. For models I these average displacements are 0.10 Å/atom,
ξ-mixed configurations for the ground states of all structures that were generated. This clearly shows that all potential models can stabilize 0.08 Å/atom for model II and 0.11 Å/atom for model III. All models are having difficulties with the energies of structures that contain less than 9 or more than 10 atoms per PMI (eV/atom) Model I Model II Model III

| Number of atoms per PMI | \( E_{\text{ab initio}} \) (eV/atom) | \( \Delta E \) (meV/atom) |
|-------------------------|--------------------------|-----------------------------|
|                         | Model I  | Model II  | Model III  | Model I  | Model II  | Model III  |
| 8                       | -4.753  | -13       | -12        | -20      |           |            |
| 8.25                    | -4.755  | -6        | -7         | -13      |           |            |
| 8.5                     | -4.756  | -1        | -3         | -5       |           |            |
| 8.75                    | -4.757  | +3        | +2         | +2       |           |            |
| 9                       | -4.755  | +4        | +4         | +3       |           |            |
| 9.25                    | -4.747  | +1        | +1         | +1       |           |            |
| 9.5                     | -4.741  | +1        | +0         | +2       |           |            |
| 9.75                    | -4.731  | -6        | -5         | -2       |           |            |
| 10                      | -4.731  | -2        | +2         | +4       |           |            |
| 10.25                   | -4.714  | -12       | -12        | -5       |           |            |
| 10.5                    | -4.704  | -15       | -17        | -7       |           |            |
| 10.75                   | -4.692  | -19       | -21        | -13      |           |            |
| 11                      | -4.683  | -22       | -24        | -17      |           |            |

TABLE V. Cohesive energies (in eV/atom) of different optimized configurations for the \( \xi \)-phase. The energy differences \( \Delta E \) between the \( \text{ab initio} \) calculations and the respective model are given in meV/atom.

All models are having difficulties with the energies of structures that contain less than 9 or more than 10 atoms in the inner shells of the PMI clusters. This may be an indication for the mechanical instability found during the structure optimization.\(^{23}\) The energy of these structures is highly unfavorable; at elevated temperatures some atoms drifted from the outer shell to the inner shell or vice versa to achieve an inner shell with 9 or 10 aluminum atoms.

All energy differences between the \( \text{ab initio} \) and EAM calculations are smaller than 10 meV/atom for configurations ranging from 8.5 to 10 atoms per PMI cluster. This energy is considered a critical threshold for the accuracy of the potentials. Regarding the energy differences between the different structures, which are on the order of 1 meV/atom, all potentials can evidently distinguish between these different configurations.

The structure optimization in Ref.\(^{24}\) yielded four almost stable structures, which are different from the ones shown in Table V. There, not only the atoms in the inner shell are varied, but also atoms not belonging to the PMI clusters. These alterations were not done in a systematic manner, the structures will be listed in tabular form. The amount of atoms for \( \xi \)- and \( \xi' \)-phases is the same, only the arrangement of the PMI cluster columns is different. These structures were tested with the three different potentials. The results can be seen in Table VI. The two upper structures in this table are \( \xi \)-phase, the lower two structures are \( \xi' \).

| composition | \( E_{\text{ab initio}} \) (eV/atom) | \( \Delta E \) (meV/atom) |
|-------------|-----------------------------------|-----------------------------|
| \( \xi \)-228–64–12 | -4.702 | -5 | +4 |
| \( \xi' \)-228–64–12 | -4.748 | +1 | +7 |
| \( \xi' \)-224–68–12 | -4.703 | -5 | +3 |
| \( \xi' \)-224–68–12 | -4.748 | +1 | +5 |

TABLE VI. Cohesive energies (in eV/atom) of the four almost stable phases after relaxation. The energy differences \( \Delta E \) are given in meV/atom. The composition is given in numbers of aluminum, palladium and manganese atoms, in this order. All configurations have 9 aluminum atoms in the inner shell of the PMI clusters. After the relaxation with the effective potentials, all models show a very good agreement with the \( \text{ab initio} \) calculated energies. The mean displacements after the relaxation are again in the same order of magnitude as before, 0.11 Å/atom for model I, 0.08 Å/atom for model II and 0.15 Å/atom for model III. Based on these pure energy comparisons, all three potential models seem to be of equal quality, with slight advantages for model III.

B. Tests

A force-matched potential is only useful, if it can reproduce key quantities that were not directly included in the reference data. Here, we subjected the three potentials to a series of tests. The first test is whether the potential can stabilize the \( \xi \)-phase even at elevated temperatures. As there was a large number of high temperature \( \text{ab initio} \) MD simulations included in the optimization, the potentials should be able to preserve the structure...
of the ξ-phase under these conditions. We carried out
an ab initio MD simulation at 1200 K for 50 ps\[^{24}\] where
the phase is still mechanically stable. In a time-averaged
picture of the density, the atoms in the two outer shells
of the PMI clusters did not move, but the atoms in the
first shell showed some rotational degree of freedom.

All three models were able to stabilize the structure
at this temperature. While models II and III give the
same results as the ab initio calculation (cf. Ref.\[^{24}\]),
model I shows additional degrees of freedom. In the time-
averaged picture the atoms forming the outer shell of the
PMIs are not as steady as in the ab initio simulation.
Also the atoms, which do not belong the these clusters,
show a density distribution that is twice as large as
expected. This means that model I may have difficulties
stabilizing the structure at even higher temperatures or
against fluctuations in the local atomic arrangement.

For molecular dynamics simulations, the stabilization
of different phases can be a problem. We checked some
well known phases for all three potential models with re-
spect to cohesive energy and phase stability. The results
can be seen in Table VII. All three potentials can sta-
bilize the different phases. The deviation of the atomic
positions after relaxation compared to the ab initio ref-
ence values is very small. The energies are reproduced
with errors of under 200 meV/atom.

Another important test is the calculation of formation enthalspes \(\Delta H\) with the potentials. \(\Delta H\) is defined as the
energy difference of a structure to the tie plane of the
pure element energies. This has been calculated for all
configurations in Tables V and VI. The reference energies
are given in Table VIII. For the structures with different
amounts of aluminum atoms in the inner shell of the PMI
clusters, the results can be seen in Figure 3. The devi-
ations from the ab initio enthalpies are very similar to
those from Table VIII. For less than 8.5 and more than 10
atoms in the inner shell of the PMI clusters the enthalpies
differ more than 10 meV/atom.

The enthalpies for the four almost stable structures are
shown in Table IX. All three models give very accurate
enthalpies with deviations all smaller than 10 meV/atom.

During the structure optimization a very long ab ini-
tio MD run with 50 000 steps at 1200 K was performed.
Snapshots were taken from this simulation at different
timesteps and quenched very rapidly. This has also been
done with the EAM potentials. The results show a very
good agreement for different snapshots. The structures
only differ very slightly in atomic positions. While there
is a steady offset of about 100 meV/atom in the energy
for higher temperatures, the overall trend can clearly be
followed. For lower temperatures and \(T = 0\) the energies
were in the same order as for the structures in Table VIII.
There were no major differences for all three potential
models.

To determine if a structure is thermodynamically sta-
 ble, the energy difference of this structure to the convex
hull is calculated. If this difference is negative, the struc-
ture is stable, otherwise it is unstable. For more details
on the convex hull see Ref.\[^{24}\]. This energy difference
has been calculated for all structures in Table V and is
shown in Fig. 4.

For the sake of clarity, the datapoints of model I and
II are shifted by +10 and +5 meV/atom. While these
models show a clear decrease of the energy difference
with increasing number of atoms inside the PMi clus-
ter, model III has minima for 9 and 10 atoms, like the ab
initio reference calculation. As this is the main criterion
for performing a structure optimization, models I and II
cannot be used for this purpose. Only model III is able
to reproduce the shape of the ab initio calculation.

The melting point for the ξ-phase has been determined
with all three potential models. In MD simulations the

![Diagram 1](image1.png)

**FIG. 3.** Comparison of the ab initio formation enthalpy \(\Delta H\)
in eV/atom) with the three potential models. The lines between
the ab initio datapoints are added as a guide to the eye.

![Diagram 2](image2.png)

**FIG. 4.** Difference of the cohesive energy to the convex hull
for different amounts of aluminum atoms in the inner shell of the
PMI clusters. The datapoints for model I are shifted by
+10 meV/atom and by +5 meV/atom for model II.
elastic constants. All Ξ-phases have an orthorhombic structure. All Ξ-phases are in the expected temperature range. The mean square displacements (Δx) after relaxation are given in Å/atom. A displacement of 0 means the value is smaller than 10⁻⁴ Å/atom.

The Al–Pd–Mn potentials presented are very well reproduced by model III. This clearly shows that force matched potentials are only very little agreement with the ab-initio values. Only model III can reproduce C_{11} and C_{22}. All other elastic constants differ by up to a factor of 3. The potentials are apparently not able to reproduce the shear stress. However, this behavior is to be expected, if one takes into account that these potentials were generated for energy minimization purposes. For other applications, like calculating mechanical properties, an extended database, containing enough data on shears, should be used. The only samples used for these potentials, that included deformations, were high temperature ab-initio MD snapshots. These were strained along either of the cartesian axes, which are perpendicular to the periodic stacking axis of the quasicrystal. The corresponding elastic constants are C_{11} and C_{22}, which are the only ones correctly reproduced by model III.

This clearly shows that force matched potentials are limited in their applications. They give very accurate results regarding the energy and forces because they are tuned to these quantities. For other physical properties, like elastic constants, the potentials are less accurate.

### VI. SUMMARY

The Al–Pd–Mn potentials presented are very well suited to model the energetics of the Ξ-phases. They were obtained with the force-matching method, which is fitting the parameters to a large database of ab initio determined reference data. All three analytic potential models only very little agreement with the ab-initio values. Only model III can reproduce C_{11} and C_{22}. All other elastic constants differ by up to a factor of 3. The potentials are apparently not able to reproduce the shear stress. However, this behavior is to be expected, if one takes into account that these potentials were generated for energy minimization purposes. For other applications, like calculating mechanical properties, an extended database, containing enough data on shears, should be used. The only samples used for these potentials, that included deformations, were high temperature ab-initio MD snapshots. These were strained along either of the cartesian axes, which are perpendicular to the periodic stacking axis of the quasicrystal. The corresponding elastic constants are C_{11} and C_{22}, which are the only ones correctly reproduced by model III.
models tested were able to reproduce the \textit{ab initio} values of the energies with very high accuracy. The error sum of the fitting process for all three potentials is very similar, yet they show very different properties when used in MD simulations.

The differences of the models become visible when calculating energy differences like formation enthalpies or the convex hull. There, model III shows the smallest deviations and can reproduce the \textit{ab initio} values with very high accuracy. The models I and II also give very good energies differences but cannot be used to predict the stability of a structure with the calculation of the convex hull. This indicates that oscillations on two length scales, like in model III, are necessary. However, the reasons for this are unclear. For further structure determination and analysis of the metadislocations in the Ξ-phases, the model potential III will be used.

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| pair       | $C_1$     | $\eta_1$ | $C_2$     | $\eta_2$ | $k$     | $\varphi$ | $h$     |
|------------|-----------|-----------|-----------|-----------|---------|-----------|---------|
| Al-Al      | 586.4805  | 7.7670    | -0.0333   | 1.0012    | 3.7658  | 3.8484    | 1.3897  |
| Al-Mn      | 338.7250  | 7.5484    | -0.4212   | 1.9271    | 2.7530  | 0.0033    | 0.5000  |
| Al-Pd      | 981.8107  | 9.1908    | -89.9193  | 4.7322    | 0.2491  | 1.3235    | 0.6211  |
| Mn-Mn      | 3.8460    | 19.9995   | -44.5953  | 4.1469    | 1.2084  | 1.0115    | 1.5938  |
| Mn-Pd      | 12.8931   | 3.4348    | -90.3824  | 4.4851    | 1.6212  | 0.0005    | 0.5007  |
| Pd-Pd      | 6625.3081 | 9.5062    | 99.8792   | 6.1164    | 3.8088  | 2.5086    | 0.5235  |

| element    | $a_1$ | $a_2$ | $\alpha$ | $\beta$ | $h$     |
|------------|-------|-------|-----------|---------|---------|
| Al         | 0.1317| 0.0399| 2.7507    | 2.3142  | 1.9995  |
| Mn         | -1.5432| 1.0321| 1.6018    | 2.4154  | 1.9996  |
| Pd         | 0.4962| 0.7317| 2.9972    | 3.4308  | 0.5001  |

| element    | $F_0$ | $F_1$ | $q$ |
|------------|-------|-------|-----|
| Al         | -2.9403| 0.5639| -1.3026 |
| Mn         | -1.5862| 1.3917| -5.3935 |
| Pd         | -4.0016| 0.9432| -5.7749 |

**cutoff radius $r_c = 7$ Å**

**TABLE XI.** Parameters for the model III EAM potential with $r$ in units of Å and $V(r)$ in eV.

**FIG. 5.** (color online) Plots of the 12 functions of the EAM potential (model III) for Al–Pd–Mn.