



## Finite element modeling of interdiffusion phenomena in solid metals

### *Modélisation éléments finis des phénomènes d'interdiffusion dans les métaux à l'état solide*

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#### ABSTRACT

A Lagrangian approach is proposed for modeling interdiffusion phenomena in solid metals. In the first section, a formulation of diffusion equations in terms of mass fraction is developed. The specificity of this approach lies in the choice of the convection velocity. In this work, it is defined as being equal to the massic average velocity. An interdiffusion strain rate tensor is also proposed to model the mass movements induced by interdiffusion phenomena. In the second section, a finite element procedure is proposed to simulate the coupled problem which includes diffusion equations and momentum balance. A one-dimensional example is presented to show the relevance of the approach developed for an interdiffusion couple.

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#### R É S U M É

Une approche lagrangienne est proposée pour modéliser les phénomènes d'interdiffusion dans les métaux à l'état solide. Dans une première partie, une formulation des équations de diffusion en fraction massique est développée. La spécificité de cette approche réside dans le choix de la vitesse de convection. Dans ce travail, elle est définie comme étant égale à la vitesse moyenne de masse. Un tenseur des taux de déformation d'interdiffusion est également proposé pour modéliser les mouvements de masse induits par les phénomènes de diffusion. Dans une seconde partie, une technique éléments finis est proposée pour simuler l'ensemble du problème couplé à savoir les équations de diffusion et le bilan de quantité de mouvement. Un exemple unidimensionnel est présenté pour montrer la pertinence de l'approche proposée pour un couple d'interdiffusion.

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## 1. Introduction

The modeling of interdiffusion is a complex problem that can occur, for example, in the study of interdiffusion couples, diffusion welding or oxidation phenomena. Diffusion in solid metals can be very intense and can produce significant mass transfer. For example, this can occur during oxidation as studied by Nicolas et al. for a Ni–16Cr–9Fe alloy oxidized at 950 °C [1]. Indeed, in this example, the movements of atoms are so important that, a very high depletion of chromium is observed in the base material under the oxide layer. This can lead to the appearance of internal stresses which may

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themselves influence diffusion phenomena. Therefore, the simulation of this type of problem requires a strong coupling between diffusion modeling and stress analysis.

To date, in physico-chemistry, these phenomena are studied mainly in terms of diffusion of species by means of the first and second Fick's laws [2,3] coupled with the thermodynamic principles. For engineering, it looks more convenient to couple the diffusion phenomena with stress analysis for taking into account other mechanical effects such as, for example, residual stresses or plasticity. The coupling with the momentum balance is not evident from the kinematic point of view because the convection velocity is often taken as being equal to the average velocity of atoms regardless of their mass. However, in solid mechanics, movements are described using the mean mass velocity field.

The aim of this paper is to propose a coupled finite element approach for the coupling between interdiffusion phenomena using chemical potential gradient and the balance of momentum based on average massic velocity. All this formulation is proposed in a Lagrangian approach for solids considered as closed systems. In the first section, a formulation of diffusion equations in terms of mass fraction is developed. The specificity of this approach lies in the choice of the convection velocity. In this work, it is defined as being equal to the average massic velocity. An interdiffusion strain rate tensor is also proposed to model the mass movements induced by interdiffusion phenomena in stress analysis. In the second section, a finite element procedure is proposed to simulate the coupled problem which includes diffusion equations and momentum balance. Finally, an example is presented to show the relevance of the proposed approach.

## 2. Theory

### 2.1. Diffusion equations

The studied closed system is assumed to be composed of  $n$  chemical elements. During interdiffusion phenomena, the mass balance must be satisfied for each element  $i$ . In an arbitrary volume  $V$  fixed in the laboratory frame of reference, it is given by the following expression:

$$\int_V \frac{\partial \rho_i}{\partial t} dV + \int_S \rho_i \mathbf{v}_i \cdot \mathbf{n} dS = 0$$

In this expression,  $\mathbf{n}$  is the unit normal outward vector to the boundary  $S$ ;  $\rho_i$  is the mass of chemical element  $i$  per unit volume.  $\mathbf{v}_i$  denotes the velocity of element  $i$  in the reference frame linked to the laboratory. The local form of this law can be written as follows

$$\frac{\partial \rho_i}{\partial t} + \text{div}(\rho c_i \mathbf{v}_i) = 0 \quad (1)$$

where  $\rho = \sum_k \rho_k$  denotes the mass of all chemical elements per unit volume and  $c_i = \frac{\rho_i}{\rho}$  is the mass fraction. The flux  $c_i \mathbf{v}_i$  can be decomposed in a diffusion part and a convective part:

$$c_i \mathbf{v}_i = \mathbf{J}_i + c_i \mathbf{v} \quad (2)$$

where  $\mathbf{J}_i$  denotes the diffusion flux.  $\mathbf{v}$  is the average velocity. In mechanics,  $\mathbf{v}$  is taken as equal to the average massic velocity of all species:  $\mathbf{v} = \sum_k c_k \mathbf{v}_k$ . The sum of the diffusion fluxes  $\mathbf{J}_i$  is then equal to zero. The diffusion equation for a species  $i$  is obtained by rewriting Eq. (1) as follows

$$c_i \left( \frac{\partial \rho}{\partial t} + \text{div}(\rho \mathbf{v}) \right) + \rho \left( \frac{\partial c_i}{\partial t} + \mathbf{v} \cdot \text{grad} c_i + \text{div}(\mathbf{J}_i) + \mathbf{J}_i \cdot \frac{\text{grad} \rho}{\rho} \right) = 0$$

Considering the total mass conservation of all chemical elements, the first term is equal to zero. The diffusion equation in terms of mass fraction is then given by

$$\frac{dc_i}{dt} + \text{div}(\mathbf{J}_i) + \mathbf{J}_i \cdot \frac{\text{grad} \rho}{\rho} = 0 \quad (3)$$

where  $\frac{d}{dt} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \text{grad}$  is the Lagrangian derivative linked to the material movement satisfying the momentum balance.

### 2.2. Diffusion fluxes

In metallic systems, the diffusion volumic flux of each chemical element  $i$  is proportional to the diffusion coefficient  $D_i$  and to the gradient of the chemical potential  $\mu_i$ . They are not necessarily such as their sum is equal to zero. Thence, arises a net flux of material which can vary in space and time. For a mechanism of diffusion involving point defects such as vacancies, there is a flux of vacancies  $\mathbf{q}^v$ . One can note that vacancies differ fundamentally from chemical species because they have no mass and they can be created or annihilated locally quasi-instantaneously. Assuming that the number of sites occupied by atoms or vacancies per unit volume is constant [2], the sum of all diffusion fluxes with  $\mathbf{q}^v$  is such that

$$\operatorname{div}\left(\mathbf{q}^v - \sum_k D_k \mathbf{grad} \mu_k\right) = \operatorname{div}(\mathbf{q}^v) - \mathcal{R}^v = 0$$

where  $\mathcal{R}^v$  denotes the source of vacancies which represents the rate of gain or lost of volume due to interdiffusion phenomena. One can note that the hypothesis of a constant number of sites is not correct when the molar volume varies significantly with the composition. Nevertheless, when this hypothesis can be acceptable, it allows to obtain easily the expression of the flux of vacancies since, without rigid body motion,  $\mathbf{q}^v$  is given by

$$\mathbf{q}^v = \sum_k D_k \mathbf{grad} \mu_k \quad (4)$$

The interdiffusion volumic fluxes  $\mathbf{q}_i$  can then be defined by the bi-velocity (Darken) method which is commonly accepted in materials science to represent the Kirkendall shift in solids [4–6]. The bi-velocity concept is based on the division in two parts of the interdiffusion volumic flux; a first one which depends on the chemical potential gradient and is independent of the choice of the reference frame and a second one which is due to the imbalance of diffusion fluxes:

$$\mathbf{q}_i = -D_i \mathbf{grad} \mu_i + f_i \mathbf{q}^v \quad (5)$$

where  $f_i$  represents the volume fraction such that  $\sum_k f_k = 1$ . In the reference frame of the laboratory, the volumic flux  $f_i \mathbf{v}_i$  of the species  $i$  is not only due to interdiffusion phenomena. Indeed, without interdiffusion, the volumic flux of the material can be caused by elasto-plastic strains involved by stresses in solid metals. Assuming an additive decomposition of the volumic flux with a first part composed of the interdiffusion volumic flux and a second part influenced by elasto-plastic strains, we get

$$f_i \mathbf{v}_i = \mathbf{q}_i + f_i \mathbf{v}^* = -D_i \mathbf{grad} \mu_i + f_i \mathbf{q}^v + f_i \mathbf{v}^* \quad (6)$$

where  $\mathbf{v}^*$  corresponds to the material velocity due to elasto-plastic strains. Therefore, the massic flux  $c_i \mathbf{v}_i$  can be expressed in terms of chemical potentials by multiplying this expression with the ratio  $\frac{c_i}{f_i} = \frac{\sum_l c_l \Omega_l}{\Omega_i}$  where  $\Omega_i$  denotes the massic volume of the chemical element  $i$ :

$$c_i \mathbf{v}_i = \mathbf{Q}_i + c_i \mathbf{v}^*$$

where

$$\mathbf{Q}_i = \left( \frac{\sum_l c_l \Omega_l}{\Omega_i} \right) \mathbf{q}_i$$

$\mathbf{Q}_i$  denotes the interdiffusion massic flux of element  $i$ . The sum of all the massic fluxes leads to the following expression of the average massic velocity:

$$\mathbf{v} = \mathbf{v}^d + \mathbf{v}^*$$

where

$$\mathbf{v}^d = \sum_k \mathbf{Q}_k$$

$\mathbf{v}^d$  denotes the mass drift velocity resulting from the combined effect of the assumption of a constant number of sites per unit volume and of the difference of massic volumes  $\Omega_i$ . In this expression,  $\mathbf{Q}_i$  can be expressed in terms of chemical potentials by combining Eqs. (4) and (5):

$$\mathbf{Q}_i = - \sum_k \tilde{D}_{ik} \mathbf{grad} \mu_k \quad \text{with} \quad \tilde{D}_{ik} = \left( \frac{\sum_l c_l \Omega_l}{\Omega_i} \right) (\delta_{ik} - f_i) D_k \quad (7)$$

where  $\delta_{ik}$  denotes the Kronecker symbol. As a consequence, the diffusion flux  $\mathbf{J}_i$  can be expressed by means of Eq. (2) as follows

$$\mathbf{J}_i = - \sum_k D_{ik}^* \mathbf{grad} \mu_k \quad \text{with} \quad D_{ik}^* = \sum_l (\delta_{il} - c_i) \tilde{D}_{lk} \quad (8)$$

2.3. Interdiffusion strain rate

The momentum balance is governed by the following expression:

$$\mathbf{div} \sigma = \mathbf{0}$$

where  $\sigma$  is the Cauchy stress tensor. In a Lagrangian approach, its time derivative  $\hat{\sigma}$  linked to the mass movement is assumed to depend linearly to the elastic strain rate tensor  $\mathbf{D}^e$  by means of the fourth rank elastic tensor  $\mathbf{C}$  as follows

$$\hat{\sigma} = \mathbf{C} : \mathbf{D}^e$$

In the context of large strain, this hypothesis corresponds to a hypoelastic behavior where  $\hat{\sigma}$  can be defined by the Jaumann derivative of the form

$$\hat{\sigma} = \dot{\sigma} - \mathbf{\Omega} \cdot \sigma + \sigma \cdot \mathbf{\Omega}$$

where  $\mathbf{\Omega}$  denotes the rotation rate tensor of the material and  $\dot{\sigma}$  is the derivative of  $\sigma$  in time without taking into account the possible rotation of the material. Just like the majority of classical elasto-plastic models for solid metals in large strain, the proposed approach is based on the assumption of additive decomposition of the strain rate into elastic and plastic parts added to a contribution due to interdiffusion phenomena,  $\mathbf{D} = \mathbf{D}^e + \mathbf{D}^p + \mathbf{D}^d$ . We shall not insist on these standard considerations.  $\mathbf{D}^p$  is the rate of plastic deformation given by the constitutive model.  $\mathbf{D}^d$  is the rate of interdiffusion strains which models mass movements. We propose to define  $\mathbf{D}^d$  with the symmetric part of the gradient of the mass drift velocity  $\mathbf{v}^d$  as follows

$$\mathbf{D}^d = \frac{1}{2} (\mathbf{grad}(\mathbf{v}^d) + \mathbf{grad}^T(\mathbf{v}^d)) \tag{9}$$

The thermodynamic equilibrium is assumed to be taken into account through the material behavior contrary to the works of Danielewski and Wierzba [6] which consider explicitly the thermodynamic principles.

3. Finite element modeling

From the simulation point of view, a staggered approach must be used to take into account the interactions between interdiffusion phenomena and mechanics. Thus the solution at each time step starts with the diffusion analysis which is followed by the mechanical analysis. The main difficulty for the numerical modeling lies in the finite element simulation of diffusion which is detailed in this section.

3.1. Strong formulation of the diffusion problem

In this paper, the chemical potentials are taken equal to the mass fraction for each chemical element for more convenience. Therefore, the strong Lagrangian formulation for diffusion phenomena in a closed material system  $\Omega$  composed of  $n$  chemical elements with boundary  $\partial\Omega$  can be written as follows:

Find  $c_i$  and  $\mathbf{Q}_i$  defined on  $\Omega \times [0, T]$  verifying the initial-boundary value problem given by

$$\left\{ \begin{array}{ll} \mathbf{div} \left( \sum_k D_{ik}^* \mathbf{grad} c_k \right) + \sum_k D_{ik}^* \mathbf{grad} c_k \cdot \frac{\mathbf{grad} \rho}{\rho} = \frac{dc_i}{dt} & (i = 1, \dots, n) \text{ in } \Omega \\ - \sum_k \tilde{D}_{ik} \mathbf{grad} c_k = \mathbf{Q}_i & (i = 1, \dots, n) \text{ in } \Omega \\ J_i^{(p)} + \lambda_i (c_i^{(p)} - c_i) = -\mathbf{J}_i \cdot \mathbf{n} & (i = 1, \dots, n) \text{ on } \partial\Omega \\ \sum_k (J_k^{(p)} + \lambda_k (c_k^{(p)} - c_k)) = 0 & \text{on } \partial\Omega \end{array} \right. \tag{10}$$

with the initial conditions

$$c_i(t = 0) = c_i^0 \quad (i = 1, \dots, n) \tag{11}$$

In these equations the  $J_i^{(p)}$ 's are prescribed "input diffusion fluxes"; the  $c_i^{(p)}$ 's are prescribed values; and the  $\lambda_i$ 's are "transfer coefficients".

One can note that the two first equations of this problem are not strongly coupled. Indeed, the only unknown variables are the mass fractions in the first equation (10)<sub>1</sub> corresponding to the diffusion equation (3) and, in the related boundary conditions (10)<sub>3</sub> and (10)<sub>4</sub>. Therefore, building an approximation of the mass fraction fields by means of standard finite elements allows to compute the mass fractions, their gradient and then, the interdiffusion massic fluxes at Gauss integration points with Eq. (7). Unfortunately, this is not sufficient for the mechanical coupling which needs to compute the strain rate

tensor  $\mathbf{D}^d$  based on the gradient of the interdiffusion massic fluxes. This is the reason why we introduce the second equation where the interdiffusion massic fluxes  $\mathbf{Q}_i$  are considered as unknowns of the problem. In this way, they are approximated with standard finite elements which allow to compute their gradients.

### 3.2. Weak formulation and numerical solution strategy

For the finite element simulation of diffusion, the weak formulation is obtained by multiplying respectively Eqs. (10)<sub>1</sub> and (10)<sub>2</sub> by some weighting functions  $c_i^*$  and  $\mathbf{Q}_i^*$  and by integrating over the domain  $\Omega$ . Integrating the first equation by parts and accounting for the boundary condition (10)<sub>3</sub>, one thus obtains the following weak formulation of the problem:

Find functions  $c_i, \mathbf{Q}_i$  such that for all functions  $c_i^*, \mathbf{Q}_i^*$ ,

$$\left\{ \begin{aligned} & \int_{\Omega} \frac{dc_i}{dt} c_i^* dV + \int_{\Omega} \sum_k D_{ik}^* \mathbf{grad} c_k \cdot \left( \mathbf{grad} c_i^* - \frac{\mathbf{grad} \rho}{\rho} c_i^* \right) dV + \int_{\partial\Omega} \lambda_i c_i c_i^* dS \\ & - \int_{\partial\Omega} (J_i^{(p)} + \lambda_i c_i^{(p)}) c_i^* dS = 0 \end{aligned} \right. \quad (i = 1, \dots, n) \quad (12)$$

$$\int_{\Omega} \left( \mathbf{Q}_i + \sum_k \tilde{D}_{ik} \mathbf{grad} c_k \right) \mathbf{Q}_i^* dV = 0 \quad (i = 1, \dots, n)$$

The finite element approximations are of the form:

$$c_i(\mathbf{x}) = \sum_{p=1}^N c_{ip} N_p(\mathbf{x}) \Rightarrow \frac{dc_i}{dt}(\mathbf{x}) = \sum_{p=1}^N \frac{dc_{ip}}{dt} N_p(\mathbf{x}); \quad \mathbf{Q}_i(\mathbf{x}) = \sum_{p=1}^N \mathbf{Q}_{ip} N_p(\mathbf{x}) \quad (13)$$

In these expressions  $N$  denotes the number of nodes.  $c_{ip}$  and  $\mathbf{Q}_{ip}$  are the values of  $c_i$  and  $\mathbf{Q}_i$  at node  $p$ .  $N_p(\mathbf{x})$  is the shape function associated to this node. In this paper, only linear finite elements are considered such as recommended by Feulvarch et al. [7] and Dalhuijsen and Segal [8] for non-linear diffusion problems. For the resolution, the principle of the staggered approach consists in computing successively  $c_i^{t+\Delta t}$  and  $\mathbf{Q}_i^{t+\Delta t}$  on the geometry at time  $t$ . Then, the mechanical analysis gives the new geometry, stresses and strains at time  $t + \Delta t$  using a classical incremental Lagrangian approach. The mass per unit volume is then updated for each finite element by means of the gradient of the displacements. Unfortunately, it is not sufficient for the diffusion problem which needs the gradient of the mass per unit volume. To overcome this difficulty, a finite element approximation of  $\rho^{t+\Delta t}$  is build in the same way than for the interdiffusion massic fluxes  $\mathbf{Q}_i^{t+\Delta t}$  as explained in the previous section.

### 3.3. Solution procedure for a 1D problem with 2 elements

For two elements, we have  $c_1 + c_2 = 1$  which allows to reduce the size of the numerical problem by eliminating one of the two diffusion equations. Substituting the nodal approximation (13) into the variational formulation (12)<sub>1</sub> of the problem and applying an implicit time integration [7], we obtain the following non-linear system of equations at each instant  $t + \Delta t$ :

$$\{\mathbf{R}_{c_1}\} \equiv \left( \mathbf{K} + \frac{[\mathbf{M}]}{\Delta t} \right) \cdot \{c_1(t + \Delta t)\} - \frac{[\mathbf{M}]}{\Delta t} \cdot \{c_1(t)\} - \{\mathbf{F}_{c_1}\} = \{\mathbf{0}\} \quad (14)$$

In this system  $[\mathbf{K}] \equiv (K_{p,q})_{1 \leq p,q \leq N}$ ,  $[\mathbf{M}] \equiv (M_{p,q})_{1 \leq p,q \leq N}$  and  $\{\mathbf{F}_{c_1}\} \equiv (F_{c_1,p})_{1 \leq p \leq N}$  are defined by

$$K_{p,q} \equiv \int_{\Omega^t} (D_{11}^* - D_{12}^*) \left( \frac{\partial N_p}{\partial x} - N_p \frac{1}{\rho} \frac{\partial \rho}{\partial x} \right) \frac{\partial N_q}{\partial x} dV + \int_{\partial\Omega^t} \lambda_1 N_p N_q dS$$

$$M_{p,q} \equiv \int_{\Omega^t} \delta_{pq} N_p dV$$

$$F_{c_1,p} \equiv \int_{\partial\Omega^t} N_p (J_1^{(p)} + \lambda_1 c_1^{(p)}) dS$$

The matrix  $[\mathbf{M}]$  is lumped in order to eliminate spurious oscillations in the time integration for linear elements as used in this paper. Eq. (14) is solved by a quasi-Newton iterative method and each iteration consists of solving the linear system

$$[\mathbf{K}] + \frac{[\mathbf{M}]}{\Delta t} \cdot \{\delta c_1\} = -\{\mathbf{R}_{c_1}\}$$

where  $\{\delta c_1\}$  denotes the increments of  $\{c_1(t + \Delta t)\}$  looked for.

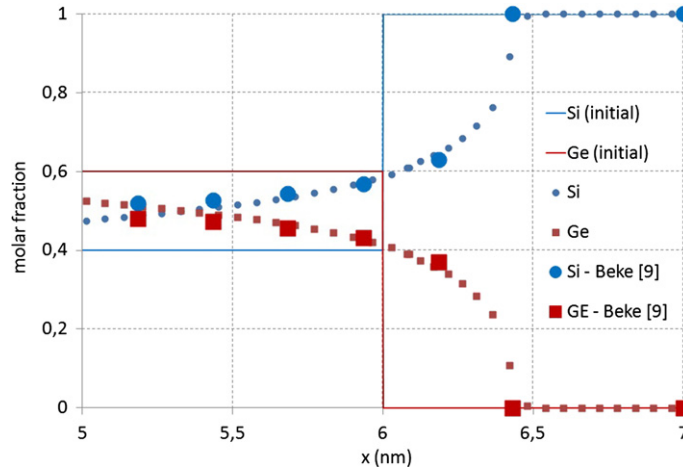


Fig. 1. Component distributions of Si and Ge, at 700 K after 2.78 h.

After convergence, the vectors  $\{\mathbf{Q}_1(t + \Delta t)\}$  and  $\{\mathbf{Q}_2(t + \Delta t)\}$  are obtained by computing the following linear system related to the weak formulation (12)<sub>2</sub>

$$\{\mathbf{Q}_i(t + \Delta t)\} = [\mathbf{M}]^{-1} \cdot \{\mathbf{G}_{Q_i}(t + \Delta t)\}$$

where  $\{\mathbf{G}_{Q_i}\} \equiv (\mathbf{G}_{Q_i,p})_{1 \leq p \leq N}$  is defined by

$$G_{Q_i,p} \equiv \int_{\Omega^t} N_p (\tilde{D}_{i_2} - \tilde{D}_{i_1}) \frac{\partial c_1}{\partial x} dV$$

After solving the diffusion problem, the geometry, the mass per unit volume and its gradient at time  $t + \Delta t$  are obtained applying a Lagrangian incremental approach in large strain considering the increment of interdiffusion strain given by

$$\Delta \epsilon^d(\mathbf{x}) = \sum_{p=1}^N \frac{\partial N_p(\mathbf{x})}{\partial x} (\mathbf{Q}_{1p}(t + \Delta t) + \mathbf{Q}_{2p}(t + \Delta t)) \Delta t$$

#### 4. 1D example

The application envisaged here involves one-dimensional modeling of the interdiffusion between pure Si and Ge at 700 K. This example is based on the one proposed by Danielewski and Wierzbka [6]. One can note that the molar volumes of these elements are different but the SiGe system has the interest to show the strong dependency of diffusivities on the mixture composition.

The volumes per unit mass  $\Omega_i$  of the components Si and Ge at 700 K are equal to:  $\Omega_{Si} = 0.286 \text{ cm}^3 \text{ g}^{-1}$  and  $\Omega_{Ge} = 0.17 \text{ cm}^3 \text{ g}^{-1}$ . In this example, the approximation proposed by Beke et al. is used for the evolution of the diffusion coefficients [9]. They are defined by  $D_{Si} = 3 \times 10^{-2} \exp(-10x) \text{ nm}^2 \text{ s}^{-1}$  and  $D_{Ge} = 4 \times 10^{-5} \exp(-10x) \text{ nm}^2 \text{ s}^{-1}$  where  $x$  equals the molar fraction of Si if it is greater than 0.5, otherwise  $x = 0.5$ . These evolutions have been obtained after numerical experiences and comparisons with the results of Beke et al.

Fig. 1 shows the component distributions obtained with a finite element mesh composed of two-node linear elements. The element size  $h$  is uniform and the time step  $\Delta t$  is invariable. The value of  $h$  is  $6 \times 10^{-2} \text{ nm}$  and a value of  $\Delta t = 50 \text{ s}$  is used. Results are plotted in terms of molar fraction as for most of profiles obtained experimentally. Fig. 2 shows the distribution of displacements after 2.78 h. This illustrates the mass movements and therefore the atom movements in the solid solution. These results show a maximal displacement at the initial position of the Kirkendall plane at  $x = 6 \text{ nm}$ . This phenomenon agrees with the Kirkendall effect in the case where the ratio of the diffusion coefficients is constant as in this example. One can note that the Kirkendall plane moves with the maximum displacement for lots of other solid solutions (FeNi, CuNi, AuCu, AuAg, ...) [2].

#### 5. Conclusion

A finite element modeling for interdiffusion phenomena in solid metals has been developed in a Lagrangian way. This is based on the coherent coupling between diffusion equations and stress analysis. A one-dimensional example has been presented to show the ability of the technique developed to model the Kirkendall effect for an interdiffusion couple. In this

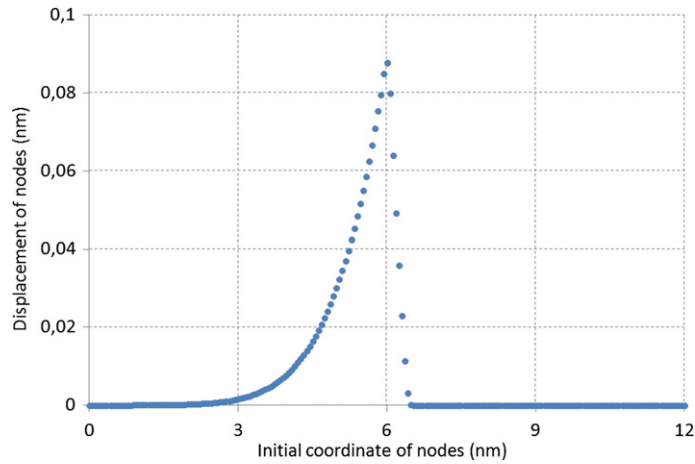


Fig. 2. Distribution of displacements at 700 K after 2.78 h.

case, one can note that stresses are always equal to zero but the technique developed can be used for multi-dimensional problems. The main difficulty lies in the knowledge of the material behavior which can depend on the mixture composition.

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