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Modeling of thermotransport phenomenon in metal alloys using artificial neural networks

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ABSTRACT

Thermodiffusion in molten metals, also known as *thermotransport*, a phenomenon in which constituent elements of an alloy separate under the influence of non-uniform temperature field, is of significance in several applications. However, due to the complex inter-particle interactions, there is no theoretical formulation that can model this phenomenon with adequate accuracy. Keeping in mind the severe deficiencies of the present day thermotransport models and an urgent need of a reliable method in several engineering applications ranging from crystal growth to integrated circuit design to nuclear reactor designs, an engineering approach has been taken in which neurocomputing principles have been employed to develop artificial neural network models to study and quantify the thermotransport phenomenon in binary metal alloys. Unlike any other thermotransport model for molten metals, the neural network approach has been validated for several types of binary alloys, viz., concentrated, dilute, isotopic and non-isotopic metals. Additionally, to establish the soundness of the model and to highlight its potential as a unified computational analysis tool, it ability to capture several thermotransport trends has been shown. Comparison with other models from the literature has also been made indicating a superior performance of this technique with respect to several other well established thermotransport models.

1. Introduction

Quantifying the mechanical and transport properties of metal alloys is important for the design and development of application specific materials. However, such a characterization is not easy since the material properties/characteristics are influenced by several factors that interact in a complex manner. In an engineering approach to tackle such complex problems, artificial neural networks (ANN) have been employed by several researchers to study the mechanical [1,2], electrical [3,4] as well as thermophysical properties of the materials [5]. ANN has also been used to study tribological properties, viz., wear rate and the friction coefficient of fiber composites [6], corrosion studies [7,8] and surface texture studies [9,10].

In this investigation, *thermotransport*, i.e., thermodiffusion phenomenon in binary metal alloys, is studied using the principles of ANN to obtain a quantitative estimate of the transport coefficient, viz., *thermotransport factor* (α). While *thermotransport* is the separation of components in an alloy subjected to non-uniform temperature, it is quantitatively given by α. Since some amount of energy is needed to dislocate and mobilize the atoms, experimental investigations often present the thermotransport phenomenon quantitatively via the *net heat of transport*, Q^*.

Thermotransport is of great significance in many applications. Among other non-isothermal systems, it plays a role in the morphological stability of the solidification front [11] and crystal growth processes [12]. It is the driving force of instability in

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the interconnect lines in an integrated chip [13]. Apart from these, thermotransport has application in the isotopic enrichment of materials, and is studied during the design of nuclear reactors that experience high temperatures [14]. Needless to say, from an engineering point of view, it is important to have an accurate quantitative measure of the thermotransport property of alloys while considering them in applications involving significant temperature gradients.

While thermotransport, also known as *thermomigration* or more generally as *thermodiffusion*, has been studied in metals [15–17], gases [18], electrolytes [19], liquid hydrocarbons [20–27], alcohols [28,29], ferrofluids [30,31], polymers [32–36], proteins [37], combustion [38], surfactant micelles [39], latex particles [40] etc., its investigation is complicated by the fact that in addition to the temperature gradient, the mixture experiencing a non-uniform thermal force is usually acted upon by one or more of the following additional forces: gravity, electric field, magnetic field, buoyancy, molecular diffusion etc. The consequent complex inter-particle interactions make the study of thermotransport very challenging. In fact, even after over a 100 years of study of thermotransport there is still no theory that can model this phenomenon accurately. So much so that in many theoretical formulations, most of these other forces are often neglected.

In the mathematical modeling of thermotransport, the starting point is the equation for diffusive flux (J) that is given in terms of the thermotransport factor or the net heat of transport as

$$J = -D\left(\nabla c + \frac{c(1-c)\alpha}{T}\nabla T\right), \tag{1}$$

$$J = -D\left(\nabla c + \frac{(1-c)Q^*}{RT^2}\nabla T\right), \tag{2}$$

where D is the molecular diffusion coefficient, ∇c and ∇T are the gradients of concentration and temperature, respectively. The above two equations are analogous to Eqs. (7) and (6), respectively, in the work of Dougherty and Drickamer [48]. The Fickian diffusion process is included in the above equation since any concentration gradient that is produced by the thermal gradient is countered by a molecular diffusion process that tries to restore the initial homogeneous state of the mixture. Comparing Eqs. (1) and (2),

$$Q^* = \alpha cRT \tag{3}$$

and from the experiments, either Q^* or α or $D_T = D\alpha/T$ or $S_T = D_T/D$ is reported.

Several theoretical approaches to study thermotransport in metal alloys can be found in the literature [17,41,42,44–46]. Among the early investigations, Lodding [45] presented the thermotransport phenomenon in terms of a separation factor, $\widetilde{S}$, that depends upon the velocities of the motion of the components of the metals. As per Lodding,

$$\nabla_T \ln \widetilde{S} = \frac{1}{\nabla T}\frac{v_1 - v_2}{D_{\text{eff}}}, \tag{4}$$

where v_i is the velocity of the species, and D_{eff} is the effective diffusion coefficient in the mixture. Further, $\widetilde{S} = \frac{(c_1/c_2)_H}{(c_1/c_2)_C}$, the subscripts H and C referring to the hot and cold side, respectively. However, this model does not account for the electronic contribution to the thermotransport process, something that is now well recognized as a non-trivial contribution.

Galina and Omini [46] proposed an enhanced model in which the authors formulated thermotransport in metals as a combination of the thermal and electronic forces. This is motivated by the fact that metals consists of ions and conduction electrons. As a result, thermotransport is a consequence of the ion-ion interactions as well as the ion-electron interactions. The former is called the intrinsic contribution or thermal contribution whereas the latter is the extrinsic or the electronic contribution that arises because of an induced electric field. In their model, the authors formulated the enrichment factor, $\widetilde{S}$, as a function of the drift velocity, w_i, that depends upon a net force F acting on a particle/ion in the mixture. More precisely,

$$F = F_{Th} + F_E, \tag{5}$$

where F_{Th} and F_E are the thermal and electronic contributions, respectively. As pointed out by Eslamian et al. [17], this model suffers from two drawbacks: (1) In the expression of the electronic contribution, several parameters might not be easily available, rendering this model quite inapplicable. (2) There is considerable debate about expression the thermal contribution as $F_{Th} = -k_B\nabla T$, k_B being the Boltzmann constant. Other investigations in metals that present thermotransport as a combination of intrinsic and extrinsic forces include the works of Balourdet and Malmejac [42], and Thernquist [16].

Thermotransport in liquid metals have also been studied using the principles of non-equilibrium thermodynamics. All the models via this approach have evolved from the pioneering works of Prigogine et al. [47] and Drickamer [48,49], who employed the theory of irreversible thermodynamics to study thermotransport in liquid mixtures. For instance, Winter and Drickamer [44] presented a thermodiffusion model along the principles of non-equilibrium thermodynamics. Their expression for the thermotransport factor is

$$\alpha = \frac{M_2\overline{V}_1 + M_1\overline{V}_2}{2\overline{M}x_1(\partial\mu_1/\partial x_1)}\left[\frac{E_1^{visc}}{\overline{V}_1} - \frac{E_2^{visc}}{\overline{V}_2}\right], \tag{6}$$

where $M_i, \overline{V}_i$ and E_i^{visc} are the molecular weight, partial molar volume and the activation energy of the ith component. Further, $\overline{M} = M_1x_1 + M_2x_2$. In proposing the above expression, the authors approximated the heat of transport for a component