AN IMPROVED MODEL TO DETERMINE THE COOLING RATES OF MESOSIDERITES AND IRON METEORITES. J. Yang and J. I. Goldstein, College of Engineering, University of Massachusetts, Amherst, MA 01003, USA (jiyang@ecs.umass.edu and jig0@ecs.umass.edu).

Introduction: Data on the Ni concentration and distribution in kamacite (α) and taenite (γ) of meteoritic metal can be used to determine the cooling rates of meteorites. Several metallographic cooling rate methods have been used to determine the cooling rates of meteorites and have been recently reviewed [1]. The reliability of these models depends on the accuracy of the phase diagram and diffusion coefficients in Fe-Ni alloy systems. This paper reports a major revision to the Hopfe and Goldstein computer model [1] for kamacite growth in meteoritic Fe-Ni metal using the latest Fe-Ni phase diagram [2] and interdiffusion coefficient data [3]. The improved model is used to determine the cooling rates of the mesosiderites and the Toluca iron meteorite.

Revised Model Parameters: *Phase Diagram*. The latest Fe-Ni phase diagram has been assessed experimentally by Yang et al. [2] as shown in Fig. 1. The major revision in the phase diagram is in the region below 400 °C. At around 400 °C, the monotectoid reaction, $\gamma_1 \rightarrow \alpha+\gamma_2$, occurs, where γ_2 is a high Ni ferromagnetic fcc phase which transforms to ordered FeNi γ" at around 320 °C. In the equilibrium diagram, around 345 °C, a eutectoid reaction, $\gamma_2 \rightarrow \alpha+\gamma'$, occurs, where γ′ is ordered Ni_3Fe.

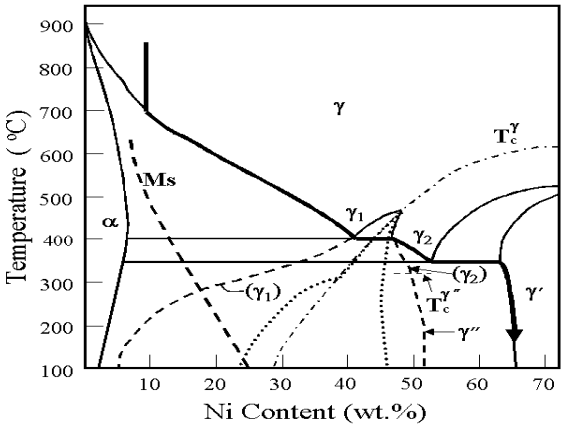

Figure 1. Fe-Ni phase diagram [2]. The (α+γ)/γ interface taenite composition as a function of temperature is shown by the bold line.

P has a pronounced effect on the phase boundary in meteorites. We follow the same α/(α+γ) solvus line for Fe-Ni binary and Fe-Ni (P saturated) pseudo binary phase diagrams used by Hopfe and Goldstein [1]. For the (α+γ)/γ solvus line, we follow the same solvus line fit by Hopfe and Goldstein [1] at temperature above 400 °C. However, below 400 °C, instead of following the metastable γ_2 and γ" phases [1], we use the equilibrium phase diagram boundary shown by the bold line in Fig.1 for the taenite composition at the taenite/kamacite interface.

Interdiffusion coefficients. The equations for interdiffusion coefficients in taenite of binary Fe-Ni alloy have been given by several researchers. Because we use the equilibrium phases γ_2 between 400 °C and 345 °C and γ′ below 345 °C, information on interdiffusion coefficients for the Ni composition up to 65 wt% is required. We cannot use the expression developed by Hopfe and Goldstein [1] since the equilibrium γ′ has a Ni composition around 65 wt%. In this study, we use the experimental data of Goldstein et al. [4] and Dean and Goldstein [5] to refit an equation for taenite interdiffusion coefficients from 10 wt% to 75 wt% Ni.

Our recent study on influence of magnetic spin ordering on interdiffusion has shown that the interdiffusion coefficients in the ferromagnetic fcc Fe-Ni phase can deviate from the lines extrapolated from the high temperature paramagnetic phase [3]. We do not include this effect in current study, however.

Our recent understanding of the magnetic contribution to interdiffusion has make it necessary to re-evaluate the interdiffusion coefficient in kamacite below the Curie temperature. Based on the theory of magnetic contribution to diffusion in Fe-Ni, a re-evaluation of the experimental data has given a more accurate expression for the interdiffusion coefficient in kamacite [3]. The new interdiffusion coefficient in ferromagnetic kamacite is used in current study.

The effect of P on the interdiffusion coefficients in Fe-Ni is given by Dean and Goldstein [5].

Mathematical Model: Kamacite growth simulations are based on the numerical model by Hopfe and Goldstein [1]. The Murry and Landis [6] variable grid spacing technique and the Crank-Nicolson [7] approximation are used to solve the diffusion equation which describes the diffusional growth of kamacite from a matrix of taenite. The new phase diagram and interdiffusion coefficient data discussed above are incorporated in this model.

Case Study: *Application to mesosiderites.* The new computer model is used to predict the cooling rates of four mesosiderites: Pinnaroo, Emery, Esterville and Vaca Muerta. The average composition value of 9.78% Ni and 0.15%P for these mesosider-

ates and a cooling temperature range from 700 °C to 200 °C is used. The calculated results using the taenite central Ni vs. taenite half width method are shown in Fig.2. The calculated results by Haack et al. [8] and Hopfe and Goldstein [1] are also given in Fig. 2. Fig.2 shows that the cooling rates predicted by the current model of 0.25~0.5 °C/My fit the experimental data quite well. These cooling rates are higher than those predicted by Haack et al. [8] and about the same as the results obtained by Hopfe et al. [1] for the taenite half width larger than 10 μm. The most important thing is that our current model can correctly predict the cooling rates for taenite half width less than ~20 μm: a region poorly fit by Hopfe et al. [1] and not fit by Haack et al. [8]. We attribute the success of current model mainly to using the Fe-Ni equilibrium phase diagram given by Yang et al. [2] below 400 °C.

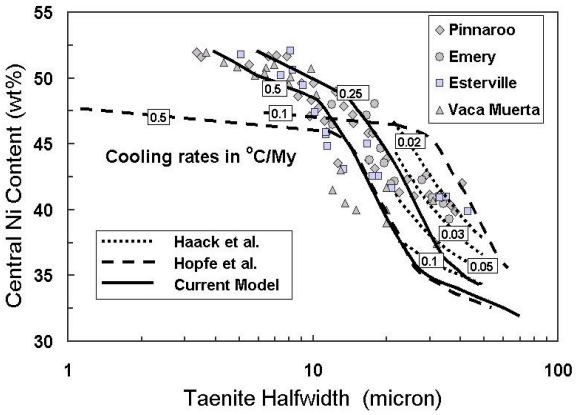

Figure 2. Central Ni content vs. taenite halfwidth for the Pinnaroo, Emery, Esterville and Vaca Muerta mesosiderites.

The central Ni vs. taenite half width data in Fig.2 can be used to explore whether γ_2/γ' or γ_2/γ'' is the reaction product at the kamacite/taenite interface below 400 °C. If γ_2/γ'' is assumed to be the interfacial reaction product, it has Ni composition around 48%-52% based on the phase diagram. Equilibrium should be maintained not only at the reaction phase interface, but also in the center region of the taenite for taenite half widths less than 10 μm where it also has Ni composition around 48%-52% based on the experimental central Ni. The low taenite interdiffusion coefficients below 400 °C make it very difficult to reach a Ni composition (~52 wt%) for the center region of the taenite. Therefore, it is not surprising that Ni contents below 52 wt% were reported for the taenite half widths less than 10 μm using the Hopfe and Goldstein model [1]. On the other hand, if γ_2/γ' is the interfacial reaction product which has a Ni composition from 48% to 53% (γ_2) between 400 °C and 345 °C, and ~65% (γ') below 345 °C, it is possible for the central Ni of taenite, less than 10 um, to reach a Ni value of 52% or more.

Application to iron meteorite. The central Ni content vs. taenite half width for a cooling rate of 25 °C/My for the Toluca iron meteorite (8.14% Ni and 0.15% P) is calculated as shown in Fig.3. The experimental data of Saikumar et al. [9] and Wood [10] as well as calculated cooling rates by Saikumar et al. [9] and Hopfe et al. [1] are also given in Fig.3. A cooling rate of 25 °C/My fits the experimental data using all three models. The central Ni content vs. taenite half width curve predicted by the current model fits the experimental data quite well, especially for taenite halfwidths less than ~10 μm.

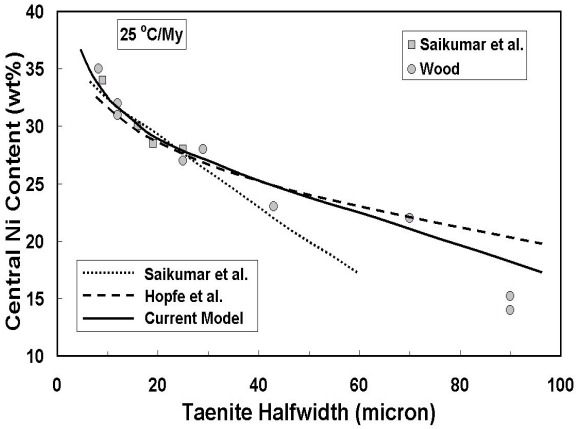

Figure 3. Central Ni content vs. taenite halfwidth for Toluca iron meteorite.

It is important to point out that cooling rates may be less than those predicted by this model, if the magnetic contribution to interdiffusion in γ_2 and γ' phases is considered. The value of the interdiffusion coefficients in γ_2 and γ' is less compared to the paramagnetic γ phase at the same Ni composition [3].

References: [1] Hopfe W. D. and Goldstein J. I., (2001) *Meteoritics & Planetary Sci., 36*, pp.135-54. [2] Yang C. W. et al. (1996) *J. Phase Equilibria, 17*, pp.522-31. [3] Yang J. and Goldstein J. I., (2003) *"Magnetic contribution to interdiffusion in bcc and fcc Fe-Ni alloys", to be submitted to Mat. & Metall. Trans*. [4] Goldstein J. I. et al., (1965) *Trans. Metall. Soc. AIME, 233*, pp.812-20. [5]. Dean D. C., and Goldstein J. I., (1986) *Metall. Trans. 17A*, pp.1131-38. [6] Murry W. D., and Landis F., (1956) *Trans. ASME J. Heat Trans*., pp.106-12. [7] Noye J. (1984) *Comp. Tech. for Diff. Equa.,* Elsevier Sci. Publ., New York, USA, p.679. [8] Haack H. et al. (1996) *Geochim. Cosmochim. Acta, 60*, pp.2609-19. [9] Saikumar V. and Goldstein J. I. (1988) *ibid, 52,* pp.715-26. [10] Wood J. A., (1964) *Icarus, 3*, pp.429-59.