

DIFFUSION IN MULTICOMPONENT SOLIDS

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PRE-REQUISITES : Preliminary knowledge of materials thermodynamics and structure of materials is desirable **INTENDED AUDIENCE :** Metallurgical Engineering, Materials Science, Mechanical Engineering, Chemical Engineering **INDUSTRIES APPLICABLE TO :**

The industry working on design and development of alloys and processes may benefit from this course e.g. to name a few are General Electrics, General Motors, Tata Steel, Boing etc.

COURSE OUTLINE :

Diffusion is the fundamental process controlling most of the phase transformations and hence, is of great interest through both theoretical and application perspectives. Knowledge of diffusion behavior of materials is essential for control as well as design of new processes. Moreover, most of the industrially important systems are based on three or more components and thus, the understanding of diffusion in multicomponent systems is particularly of greater interest. This course will treat both the phenomenology and atomic theory of diffusion in multicomponent systems. In most of the first half, the course will cover the phenomenological aspect of diffusion, which is more important practically as it deals with usage of phenomenological diffusion coefficients for modeling various diffusion-driven processes as well as actual determination of these coefficients. Major part of the later half will focus on understanding the theoretical aspect of diffusion including atomic mechanisms of diffusion, fundamental driving forces for diffusion and dependence of phenomenological diffusion coefficients on atomic jump frequencies and thermodynamic factors. All the concepts and treatments will be explained in the context of both binary and multicomponent effects in diffusion. At the end of the course, the student should be able to describe diffusion in dilute as well as concentrated multicomponent alloys in terms of multicomponent diffusion coefficients, solve the diffusion equation for various processes, identify the various types of diffusion coefficients and select the appropriate type for a given model, understand the physical significance of these coefficients, evaluate these coefficients theoretically for some model systems and know the various methodologies of their experimental determination.

ABOUT INSTRUCTOR :

Prof. Kaustubh Kulkarni finished his PhD from Purdue University on the topic of multicomponent diffusion. He worked in Industry for four years before joining IIT Kanpur in 2012. His research mainly focusses on understanding of multicomponent effects in diffusion kinetics and applying those for designing advanced materials and processes. The cross effects in diffusion mainly originate from thermodynamic interactions and hence, developing correlations between the multicomponent diffusion effects and thermodynamic properties is an integral part of my research. While working on this, he have developed a passion for teaching both Materials Thermodynamics and Diffusion in Solids. This course is an attempt to take the multicomponent effects in diffusion, which so far have been discussed only within restricted community of researchers working on diffusion, to the broader audience of metallurgical and materials engineering.

COURSE PLAN:

Week 1: Basics of thermodynamics: laws of thermodynamics, concept of chemical potentials and criteria for equilibrium

Week 2: Refresher on Solution Thermodynamics and Phase Stability

Week 3: Phenomenology of multicomponent diffusion and various frames of reference used for measuring diffusion fluxes

Week 4: Solving diffusion equation for various boundary conditions including solution of multicomponent diffusion equation

Week 5: Self diffusion, impurity diffusion, interdiffusion and intrinsic diffusion; Experimental determination of interdiffusion and intrinsic diffusion coefficients

Week 6: Point defects in crystalline solids and mechanisms of diffusion

Week 7: Random walk, diffusivity and correlation effects in diffusion

Week 8: Derivation of correlation factors in some crystalline lattices

Week 9: Derivation of fundamental driving forces for diffusion: chemical potential gradients and atomic mobilities; cross effects in multicomponent diffusion driven by defect mechanisms

Week 10: Interrelation between multicomponent diffusion coefficients, atomic jump frequencies and thermodynamic factors

Week 11: Multiphase diffusion, diffusion structures and phase diagrams

Week 12: Experimental determination of activation energies for diffusion; Fast diffusion paths: Grain boundary and pipe diffusion