**Name of the module: Grain Boundary Segregation and Fracture of Materials**

**Number of the module:365/2/6954**

**Number of module: 365-2-6011**

BGU Credits: 3

ECTS credits: 4

Academic year: 2011-2012

Semester: Autumn semester

Hours of instruction: 3 hours per week

Location of instruction: Markus

Building

Language of instruction: **English**

**All the students receive the detailed synopsis of ALL THE LECTURES in English**

Cycle: Second cycle

Position: An advanced course for graduate students in Materials Engineering Department

Field of Education: Materials Science and Engineering

Responsible department: Materials Engineering

General prerequisites: Introduction to MSE

Grading scale: the grading scale would be determined on a scale of 0 – 100 (0 would indicate failure and 100 complete success 0 to 100), passing grade is 65.

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Module evaluation: at the end of the semester the students will evaluate the module, in order to draw conclusions, and for the university's internal needs.

**Course Description:**

Materials can be intrinsically ductile (e.g. pure FCC metals), brittle (e.g. ceramics, glasses, Si) or, like many BCC metals, e.g. steels, experience ductile-brittle transition under low temperature and/or high- strain -rate loading. The otherwise confusing subject of ductile vs. brittle behavior is usually rationalized by considering it as a competition between dislocations/viscous flow processes and cracks growth. More deep insight into the problem shows however that macroscopically brittle fractures are most often microscopically ductile .These findings that cannot be understood in terms of the dilemma “ Ductile or Brittle “ shed light on the *atomistic of fracture* . Its understanding is beyond the borders of macroscopic fracture mechanics and is essential for improvement of fracture resistance of classical and novel structural materials ,in particular nano-structured and amorphous metals and ceramics of super-high strength.

 Considering now the “embrittlement “ phenomena ,even the intrinsically ductile materials , say pure Cu , can become brittle when they contain some “harmful” impurities , e.g. Sb or Bi , which segregate at grain boundaries from solid solution. So called “reversible temper brittleness” caused by presence of several ppm of P or As in high strength steels is another classical example of inter-granular fracture caused by impurity segregation . Along with *harmful* impurities, there exist also the *beneficial* ones which segregation at interfaces improves resistance to fracture. The central issues here are the atomic mechanism of equilibrium grain boundary segregation and the physics behind harmful or beneficial action of the specific impurities. These issues can be addressed now based on the helpful semi-empirical criteria and considerable progress in ab*-initio* calculations.

 Time is a factor of primary importance in mechanical behavior and wide class of impurity and environmental effects in embrittlement involves timedependent subcritical crack growth leading to delayed failures .This type of failures is often associated with impurities segregation at grain boundaries that makes the environmental effect much more severe. The well known, though still far from adequate understanding and control, phenomena which create reliability problems in nuclear energetics , welding / soldering / coating and oil/gas industry are liquid metal embrittlement (LME) and hydrogen embrittlement (HE) of metals . Another example is water induced delayed failure of rocks and glasses in such critical applications as nuclear waste depository.

 It is essential for materials engineers to understand mechanism of the impurity and environmental effects in embrittlement and delayed failures to be able to avoid them by professional material selection. Providing such an understanding is the goal of the course.

**Aims and Objectives of the module:**

**To teach student thermodynamic and kinetic aspects of equilibrium grain boundary segregation (EGBS) of impurities in polycrystalline solids and microscopic mechanisms of segregation induced intergranular fracture.**

**Learning outcomes of the module:**

On successful completion of the course the students should be able:

•to understand thermodynamics and kinetics of EGBS and make semi-quantitative estimation of it at different T, composition, grain size

•to recognize and predict effect of harmful and beneficial atomic species on GB cohesion energy

 • To understand microscopic mechanism of low temperature GB fracture

 and delayed /environmentally assisted failures

• to use this information in material selection and failure analysis

 **Attendance regulation:**

Attendance and participation in the class is mandatory (at least 80%).

**After completing the course students**

 **Attendance regulation:**

Attendance and participation in the class is mandatory (at least 80%).

**Teaching arrangement and method of instruction**: lectures, which include the examples for solving problems

Confirmation: the syllabus was confirmed by the faculty academic advisory committee to be valid on 2012-2013.

Last update: 04.09.2012

**Assignments**: three home works of about 15 problems taken together.

 **Exam** that consists of 5-6 numerical problems and conceptual questions

**Assessment:**  Exam: 75%. Home works: 25%.

**Time required for individual work**: in addition to attendance in class, the students are expected to do their assignment and individual work: at least 2 hours per week.

**Module Content and Outlines:**

**I. Fracture of Materials: Multi-scale Approach (~8 h)**

I-1. Macro- Mezo- and Microscopic Aspects: from fracture mechanics to atomistic. Intergranular fracture fields at fracture mechanism maps of solids.

I-2. Stress concentration: cracks, voids and dislocations. Cumulative vs. non-cumulative fracture. Fractography.

 I-3.Thermodynamic of fracture: chemical potential at the crack tip in the stressed solids; the Griffith criterion and its interpretation.

I-4. Ideal shear vs. ideal cleavage stresses: the criteria of inherent brittleness. Critical role of intrinsic surface energy γ. Environmental and impurity effects on γ.

I-5. Fracture as kinetic process: crack nucleation, subcritical extension and catastrophic growth; diagrams “crack velocity vs. driving forces G“; delayed failures

I-6. Dislocation mechanisms of micro-crack nucleation and extension. The Mott –Stroh vs. Hall-Petch and Griffith equations.

I-7. Energy dissipation processes at the crack tip, or why GIC >> γ: role of dislocation emission, plastic flow, voids and ligament tearing in the plastic zone

I-8. Ductile-Brittle transition; role of microstructure. Fracture and delayed failure of very brittle metals , glasses and ceramics

**II. Equilibrium Grain Boundary Segregation (EGBS) (~10h)**

II-1.Random and special grain boundaries in solids: atomic structures, elastic fields and interaction with point defects

II-2. Equilibrium and non-equilibrium grain boundary segregation of impurities: driving forces, characteristic length scales and manifestations.

II-3.Thermodynamics and kinetics of equilibrium segregation (**EGBS**) of atomic species: the GB surface coverage ϴ and interface energy γ GB; effect of temperature, concentration and pressure. Correlation with inverse solubility and its interpretations. Specific features of GBS in nano-structured solids.

**III. Mechanisms of Intergranular Brittle Fracture affected by EGBS (~8 h)**

III-1. Examples: GB micro-chemistry and fracture resistance of BCC and FCC metals. Reversible temper brittleness of steels: 100 year investigation

III-2. Effect of EGBS effect on the grain boundary cohesion energy W C; the criteria of harmful and beneficial impurities. Computer modeling and a*b-initio* calculations of EGBS and GB cohesion.

III-3. Competition for adsorption sites at GBs and improvement of GB cohesion by micro-alloying: intergranular brittleness in model alloys Fe-P –C and Cu-Sb-B

**IV. Delayed and environmentally sensitive failures** **affected by EGBS** (~ 5 h)

**V. GB Engineering to Improve Resistance to GB Embrittlement (~2 h)**

***Literature to the course:***

***1. P. Lejcek, Grain Boundary Segregation in Metals, 2010, Springer***

***2. R. Wei, Fracture Mechanics: Integration of Mechanics, Materials Science and Chemistry, Cambridge University Press, Cambridge, 2010***

***3. Fracture: An advanced treatise, ed. H. Leibowitz, v.1, Microscopic and macroscopic fundamentals, Academic Press New York***

 ***[5] 4.B. Lawn, Fracture of Brittle Solids, 2nd edition, Cambridge University Press, Cambridge, 1993***