

KATILARIN ELEKTRONİK YAPISININ BENZETİŞİMİ

Malzeme Bilimi: Temel Kavramlar

Doç.Dr. Yeşim Moğulkoç

E-posta: mogulkoc@eng.ankara.edu.tr
Tel: 0312 2033550

Hafta

DERS İÇERİĞİ

- | | |
|----|---|
| 1. | Malzeme Bilimi: Temel Kavramlar |
| 2. | İşletim Sistemleri, Temel Linux Komutlarının Uygulamalı Öğretilmesi ve
Yoğun Madde Fiziğinde Kullanılan Yazılımlar |
| 3. | Kristal Fiziği: Temel Kavramlar-1 |
| 4. | Kristal Fiziği: Temel Kavramlar-2 |
| 5. | Katlıların Bant Teorisi |
| 6. | Elektronik Bant Yapıları: İletkenlik durumları |
| 7. | VİZE SINAVI |

Hafta DERS İÇERİĞİ

- | | |
|-----|--|
| 8. | Durum Yoğunlukları ve Fermi Yüzeyleri |
| 9. | Katıların Elastik Özellikleri:
Elastik sabitleri, Young, Shear Modüller.. |
| 10. | Katıların Optik Özellikleri:
Dielektrik sabitleri, Yansıma, soğurma, sönüüm katsayıları, kırılma indisı |
| 11. | Katıların Titreşimsel Özellikleri:
Fononlar |
| 12. | Kristal yapının programlama yardımıyla kurulması |
| 13. | Katının elektronik bant yapısının programlama yardımıyla çizdirilmesi |
| 14. | FINAL SINAVI |

Malzeme Bilimi nedir?

- 1. Tanım:** Fizik ve kimyanın ortaklaşa çalışıldığı odağında malzeme olan bir bilim dalıdır.
- 2. Tanım:** Malzemelerin bileşimi ve özelliklerini inceleyen bilim dalıdır.

Malzeme Türleri

Metaller	Seramikler	Polimerler	Kompozitler
<ul style="list-style-type: none">• Alüminyum• Bakır• Çelik• Nikel• Titanyum	<ul style="list-style-type: none">• Kil• Silikon cam• Alüminyum oksit• Kuartz	<ul style="list-style-type: none">• PVC• Teflon• Çeşitli plastikler• Yapıştırıcılar• Çelik yelek	<ul style="list-style-type: none">• Tahta• Karbon fiberler• Beton

Yarıiletken malzemeler (bilgisayar çipleri, vb.): Seramik, kompozit malzemeler
Nanomalzemeler: seramikler, metaller, polimerler, kompozit malzemeler

Atomik Yapı (10^{-10} m)

* Elektronik yapı ve atomik bağlar

İyonik

kovalent

metalik

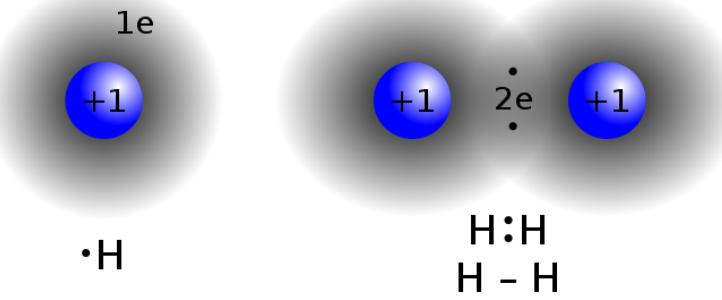
London etkileri (van der Waals)

* Atomik sıralama

7 kristal yapı – Metal ve seramikler arasında en çok kübik ve heptagonal yapılar vardır.

Toplamda 14 farklı Bravais örgüsü.

Primitive, body-centered, face-centered

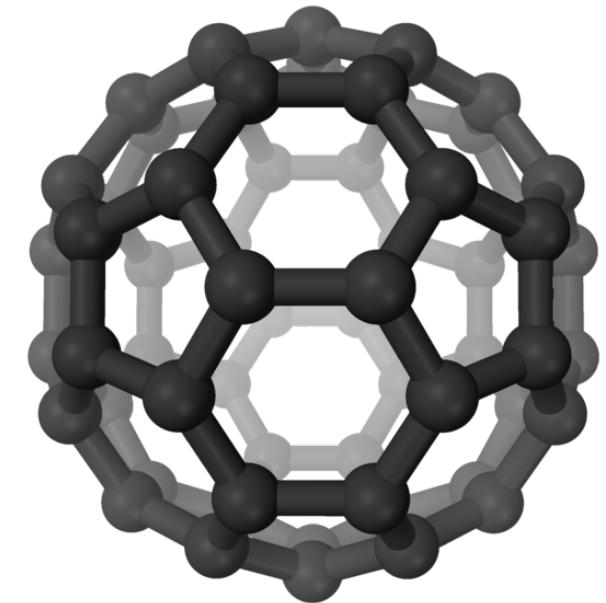


Nano yapı (10^{-9} m)

Length scale that pertains to clusters of atoms that make up small particles or material features

Show interesting properties because increase surface area to volume ratio

- More atoms on surface compared to bulk atoms
- Optical, magnetic, mechanical and electrical properties change



Mikro yapı (10⁻⁶ m)

Larger features composed of either nanostructured materials or periodic arrangements of atoms known as crystals

Features are visible with high magnification in light microscope.

- Grains, inclusions other micro-features that make up material
- These features are traditionally altered to improve material performance

Makro yapı (10^{-3} m)

Macrostructure pertains to collective features on microstructure level

Grain flow, cracks, porosity
are all examples of macrostructure features

Metaller

Metals consist of alkaline, alkaline earth, metalloids and transition metals

Metal alloys are mixtures of two or more metal and nonmetal elements (for example, aluminum and copper, Cu-Ni alloy, steel)

Bonding: Metallic

Properties:

- Electrically conductive (free electrons)
- Thermally conductive
- High strength – large capacity to carry load over x-section area (stress)
- Ductile – endure large amounts of deformation before breaking.
- Magnetic – ferromagnetism, paramagnetic
- Medium melting point

Metallerin Uygulamaları

Electrical wire: aluminum, copper, silver

Heat transfer fins: aluminum, silver

Plumbing: copper

Construction beams (bridges, sky scrapers, rebar, etc.): steel (Fe-C alloys)

Cars: steel (Fe-C alloys)

Consumer goods:

- cans
- appliances (stainless steel sheet metal)
- tools
- Many, many, many more...

Polimerler

Polymers consist of various hydro-carbon (organic elements) with select additives to elucidate specific properties

Polymers are typically disordered (amorphous) strands of hydrocarbon molecules.

Bonding: Covalent-London Dispersion Forces

Properties:

- ductile: can be stretched up to 1000% of original length
- lightweight: Low densities
- medium strength: Depending on additives
- chemical stability: inert to corrosive environments
- low melting point

Polimerlerin Uygulamaları

Car tires: vulcanized polymer (added sulfur)

Ziplock bags

Food storage containers

Plumbing: polyvinyl chloride (PVC)

Aerospace and energy applications: Teflon

Consumer goods:

- calculator casings
- TV consuls, shoe soles, cell phone casing, Elmer's Glue (adhesives), contact lenses
- Many, many. many more...

Seramikler

Consist of metal and non metal elements

Typically a mixture of elements in the form of a chemical compound , for example Al_2O_3 or glass

Three types: composites, monolithic and amorphous ceramics

Bonding covalent – ionic

- In some cases highly direction covalent bonding
- Ionic in case of SiO_2 glasses and slags



Properties:

- wear resistant (hard)
- chemical stability: corrosion resistant
- high temperature strength: strength retention at very high temperatures
- high melting points
- good insulators (dielectrics)
- good optical properties

Seramiklerin Uygulamaları

Window glass: $\text{Al}_2\text{O}_3 - \text{SiO}_2 - \text{MgO} - \text{CaO}$

Aerospace, energy and automotive industry

- heat shield tiles
- engine components
- reactor vessel and furnace linings

Consumer products:

- pottery
- dishes (fine china, plates, bowls)
- glassware (cups, mugs, etc.)
- eye glass lenses

Kompositler

Bonding: depends on type of composite (strong-covalent, medium-solid solution, weak-tertiary phase layer)

Properties: Depends on composites

- High melting points with improved high temperature strength: ceramic-ceramic
- High strength and ductile with improved wear resistance: metal-ceramic
- High strength and ductile: polymer-polymer

Kompozitlerin Uygulamaları

Wood: naturally occurring biological material consists of very strong fibers imbedded in a soft matrix

Plywood: laminated wood for buildings

Concrete: basements, bridges, sidewalks

Fiberglass: boats

Carbon fiber resins: bicycle frames

Advanced Applications Ceramics & Composites

Aerospace and Defense Applications

- Structural materials used for missiles, aircraft, space vehicles

Ultrahigh Temperature Ceramic-Composites (UHTCs)

- Metal-nonmetal, Covalent bonded compounds ($\text{ZrB}_2 - \text{SiC}$)
- High melting point materials; strong materials at temperature; excellent oxidation resistance



Why these materials?

- Service temperatures are in excess of 2000°C (~1/3 surface temperature of our sun)
- Materials have high melting points (>3000°C)
- Excellent strength retention at service temperatures
- Relative chemical stability at service temperatures
- Light weight

Other well known materials

Semiconductors – ceramics

- computer chips
- memory storage devices
- solar cells
- image screens

Nanomaterials – ceramics, metals, polymers

- gold nanoshells
- quantum dots
- medical devices