Experiment No: 01

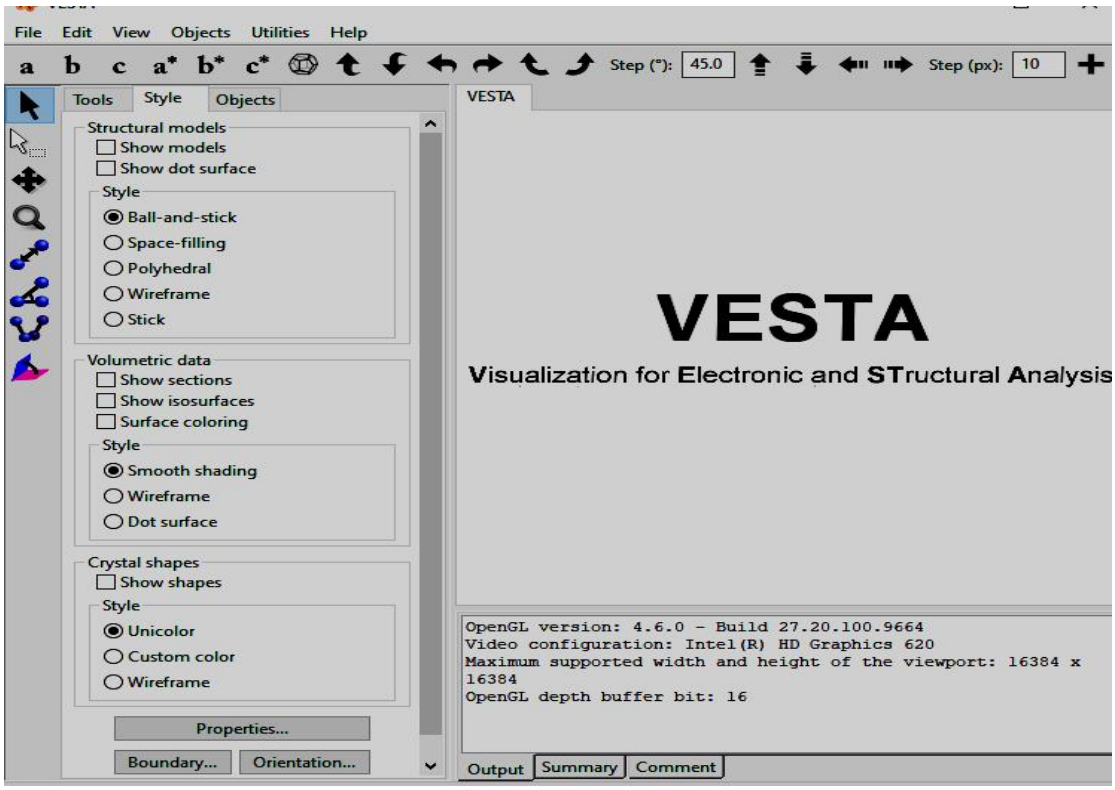
To visualize and manipulate crystallographic data and determine structural properties using software for crystalline and molecular structure (VESTA).

Abstract:

To Investigate the structural properties of crystalline and molecular solids using software (VESTA). Also visualize and manipulate the crystallographic data of a given sample.Take two crystal structures of B_2Mg (magnesium dibromide) and ZrC (zirconium carbide), then visualize and manipulate their crystallographic data using VESTA software tools .then determine their structural properties from their crystallographic data , by comparing both solid . Finally,vesta can successfully visualized and manipulate crystallographic data of B_2Mg and ZrC using VESTA software. And this analysis revealed many structural properties of both solids.

Introduction:

VESTA (visualization for Electronic and Structural Analysis) is a comprehensive software tool designed for the visualization and analysis of crystallographic data. Developed by the institute for solid state physics at the university of Tokyo, VESTA provides an intuitive and user-friendly interface for researchers to explore and understand the structural properties of crystalline and molecular solids. It enables the discovery of new materials and optimization of existing one.



Crystallography is the study of the arrangement of atoms within a crystal providing valuable insights into the materials structure, properties and behavior.
By analyzing the crystal structure we seek to determine the structural properties such as,

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Magnesium dibromide(B_2Mg)

1 . Lattice type of (B_2Mg): P

2.Lattice parameters

a	b	c	alpha	beta	gamma
3.08500	3.08500	3.52300	90.0000	90.0000	120.0000

Space Group: P 6/m m

V = 29.0371 Å^3

2. Structure parameters of

x	y	z	Occ.	U	Site	Sym.		
Mg	Mg	0.0000	0.00000	0.00000	1.000	-0.000	1a	6/m
B	B	0.33333	0.66667	0.50000	1.000	-0.000	2d	-6m2

3. Number of polygons and unique vertices on isosurface = 0 (0)
57 atoms, 84 bonds, 14 polyhedral; CPU time = 5 ms

Zirconium Carbide (ZrC):

1. Lattice type: F

2. Lattice parameters

a	b	c	alpha	beta	gamma
4.76000	4.76000	4.76000	90.0000	90.0000	90.0000

Space group: Fm - 3m

3. Structure parameters:

x	y	z	Occ.	U	Site	Sym.		
1	Zr	Zr1	0.00000	0.00000	0.00000	1.000	-0.000	4a	m-3m
2	C	C1	0.50000	0.50000	0.50000	1.000	-0.000	4b	m-3m

volume = 29.037126 Å^3

Number of polygons and unique vertices on isosurface = 0 (0)
27 atoms, 0 bonds, 0 polyhedral; CPU time = 3 ms

Lattice planes:

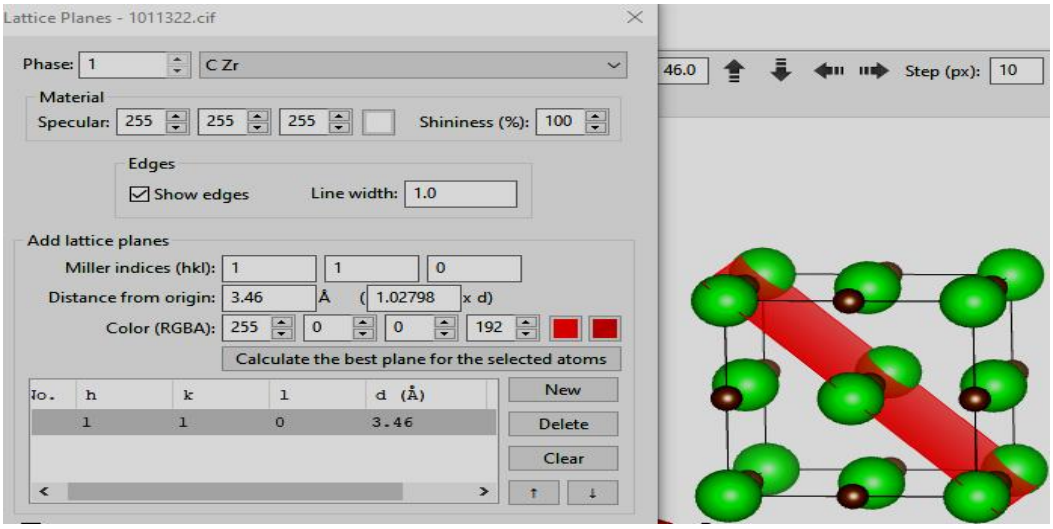
Definition A set of parallel planes that run through the lattice points of a crystal

Spacing The distance between adjacent lattice planes

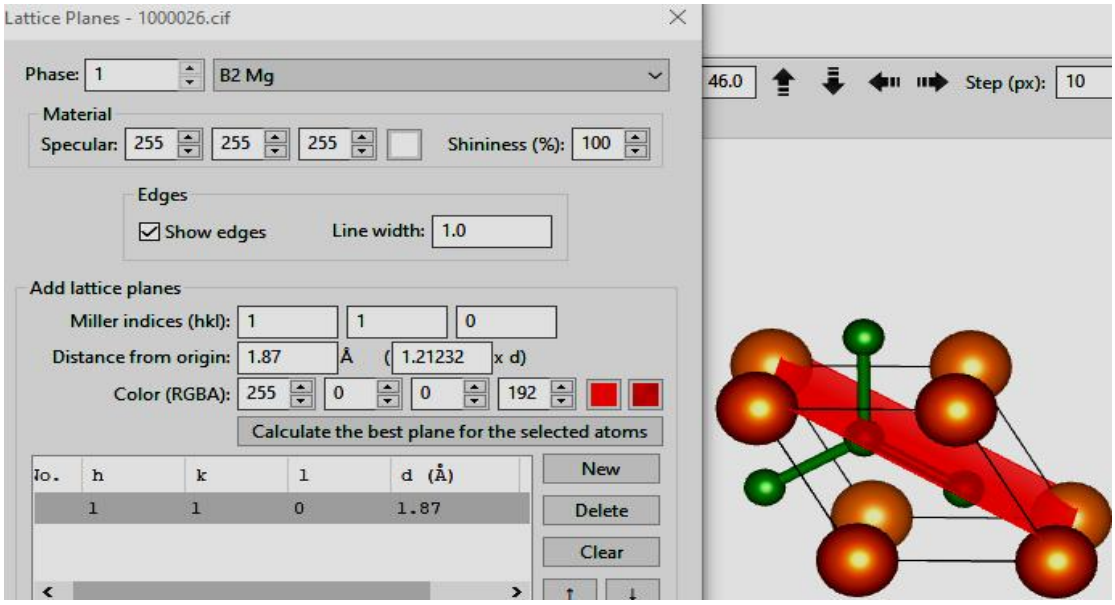
Orientation Described by Miller indices, which are sets of three integers (h,k,l)

Families Collections of equally spaced parallel lattice planes that intersect all lattice points

Zirconium Carbide:



Magnesium Dibromide:

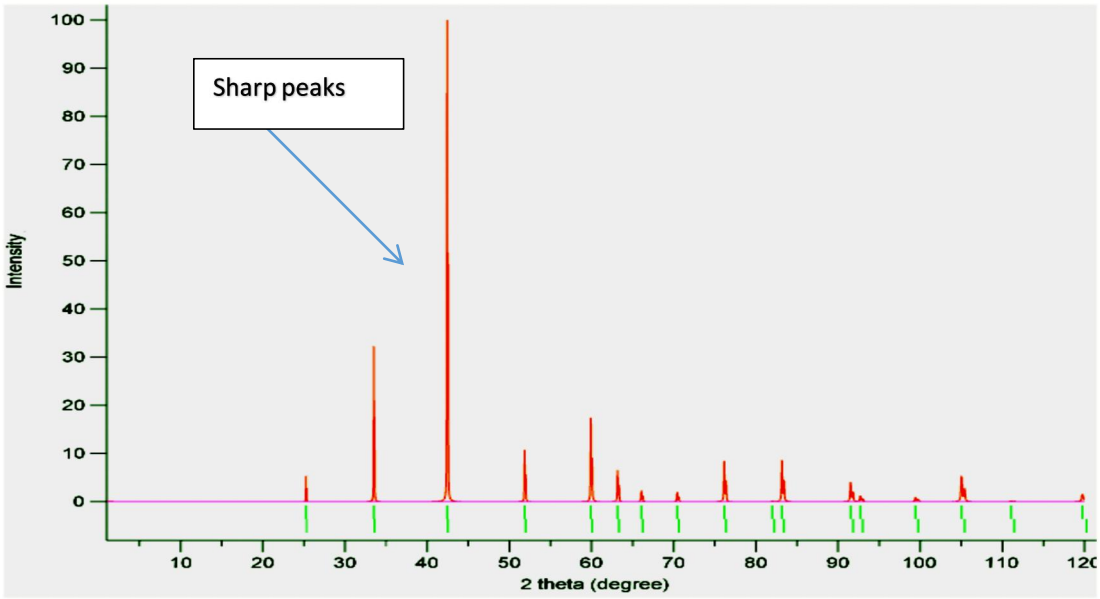


Powder diffraction pattern:

In this experiment, we also used X-ray powder diffraction pattern(XRD) to analyze the crystal structure of our crystal sample. The resulting diffraction pattern is a plot of the intensity of the diffracted X-rays versus the diffraction angle(2ɵ).It provides information about the:

1. Crystal structure :
2. Phase identification:
3. Peaks:
4. Background:
5. Peak broadening

By analyzing the powder diffraction pattern we can gain valuable insights into the crystals structures and properties of our sample.



Variation of intensity with diffraction angle (2ɵ)

Sharp peaks at specific angle (2ɵ) indicate a crystalline structure.

Equipment / Accessories:

- Compute or laptop with VESTA software installed
- Crystallographic data files (CIF)
- Crystal structure visualization tools

Experimental Design:

1. I Launch VESTA software and open the CIF file of B_2Mg and ZrC one by one.
2. I Visualize the crystal structure in 2D and 3D using various tools (rotation, Zoom).
3. Then, I manipulate the crystal structures as needed (i.e rotate,translate, scale).
4. I analyze the crystal structures using VESTA tools

- Edit
- Edit data

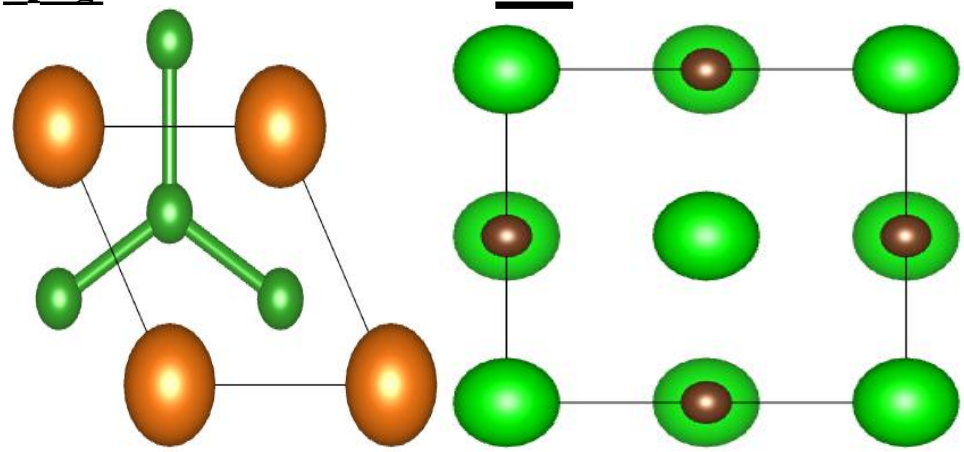
4. Then, I found following output
   Crystal system
   Bond lengths
   Bond angles
   Coordination numbers
   Space groups
   Lattice parameters

Then I get powder diffraction pattern by using VESTA tool powder diffraction pattern in Edit data menu.

5. After that I save the modified structures (raster and vector images) .
6. Finally, I Compare and contrast the results of the analysis and manipultion.
7. I also draw lattice planes (110) in both structures (ZrC, B2Mg).

Structures:

B_2Mg **ZrC**



Observations:

Peak values for B_2Mg

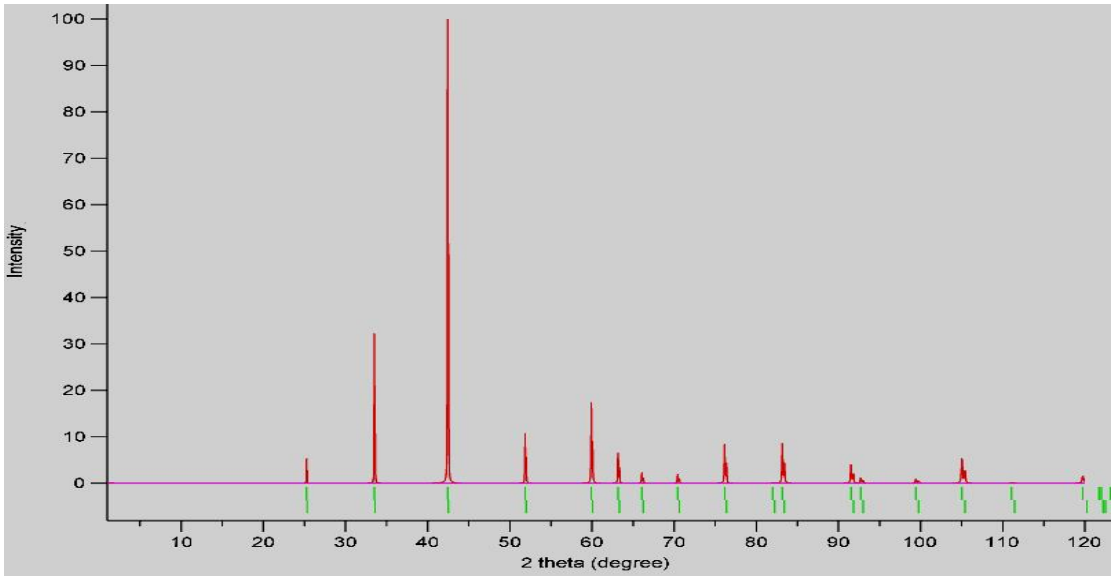
h	k	l	intensity	Diffraction angle(2ɵ)	Wavelength (m)
1	0	1	100.000	42.4275	1
1	0	1	49.7219	42.5353	2
1	0	0	27.9681	33.5146	1
1	1	0	23.9986	59.9182	1

Peak values for ZrC:

h	k	l	intensity	Diffraction Angle(2ɵ)	wavelength
1	1	1	100.00	32.555	1
2	0	0	79.587	37.768	1
2	2	0	52.274	54.4796	1
1	1	1	49.744	32.636	2

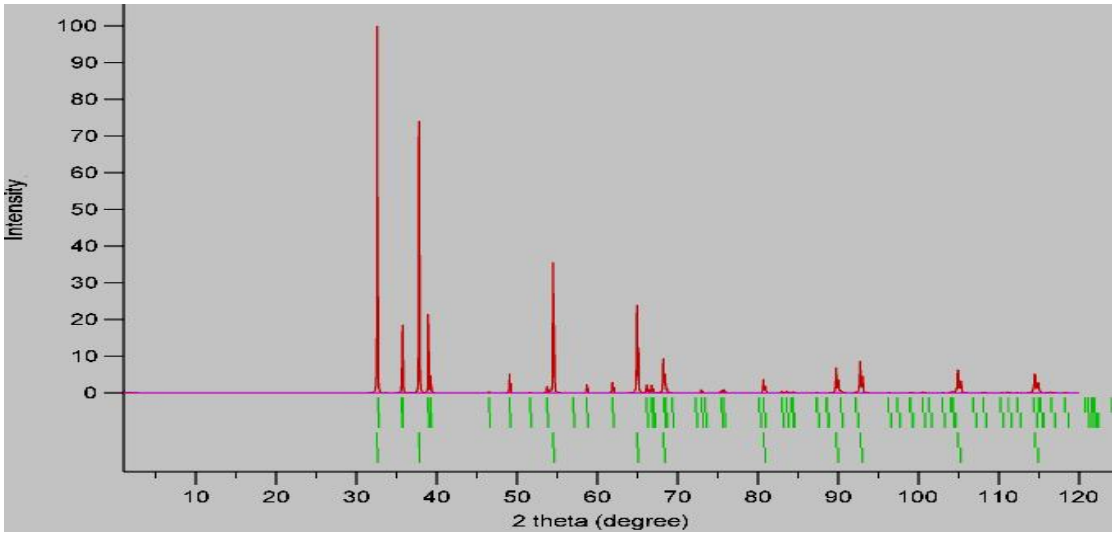
Analysis:

Powder diffraction pattern of B_2Mg:



Variation of intensity with diffraction angle(2ɵ)

Powder Diffraction pattern of ZrC:



Output:

For Magnesium dibromide:

Lattice type P
Space group name P 6/m m m
Space group number 191

Bond lengths:	Bond angles:
A = 3.08500 Å	α = 90.0000°
b = 3.08500 Å	β = 90.0000°
c = 3.52300 Å	γ =120.0000A

Unit-cell volume = 29.037126 Å^3

For Zirconium Carbide:

Lattice type F
Space group name F m -3 m
Space group number 225

Space Group: F m -3 m

Bond lengths:	Bond angles:
a = 4.76000 Å	α = 90.0000°
b = 4.76000 Å	β = 90.0000°
c = 4.76000 Å	γ = 90.0000°

Unit-cell volume = 107.850192 Å^3

Energy for Zirconium Carbide:

Radius of an ionic sphere: 3.00 Å
Reciprocal-space range: 3.00 Å**(-1)
Number of symmetry operations: 96
Number of atoms in the asymmetric unit: 2
Inversion center at the origin: 1

Electrostatic energy per asymmetric unit:

-0.243157 e**2/Å = -3.50138 eV = -0.337831 MJ/mol

Energy for Magnesium dibromide:

Radius of an ionic sphere: 3.00 Å
Reciprocal-space range: 3.00 Å**(-1)
Number of symmetry operations: 12
Number of atoms in the asymmetric unit: 2
Inversion center at the origin: 1

Electrostatic energy per asymmetric unit:

0.000000 e**2/Å = 0.00000 eV = 0.000000 MJ/mol

Conclusion:

I successfully visualized and manipulated crystallographic data for B_2Mg and ZrC crystal structures using VESTA software. And Determine the different structural properties. This analysis revealed valuable insights into the structural properties of the materials (B_2Mg, ZrC) such as lattice parameters, lattice type, unit cell parameters, Bond angles and Bond lengths and electrostatic energy per asymmetric unit.