Experiment No: 08

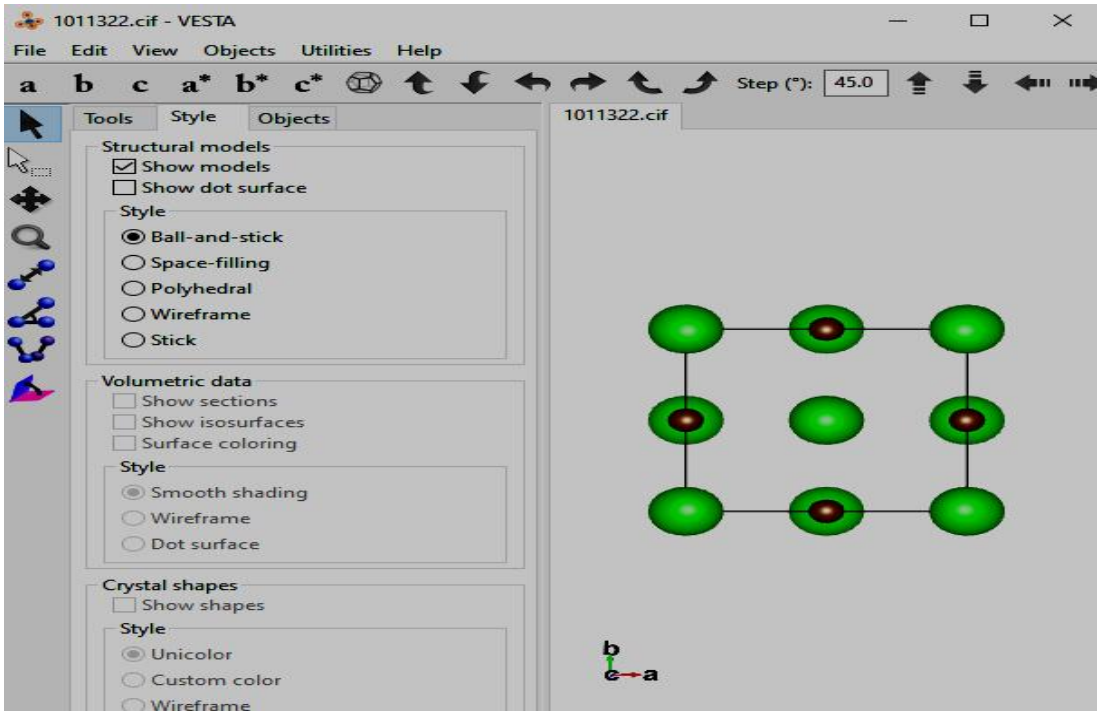
To construct and simulate point defects in solids using the supercell approach.

Abstract:

To investigate the effects of point defects (vacancies and impurities) on the electronic structure and the material properties of Zirconium Carbide (ZrC)
This experiment utilizes the super cell method to computationally construct and simulate various point defects in a crystalline solid, allowing for the analysis of their structural and electronic properties by artificially introducing vacancies, interstitials, or impurity atoms into a periodic unit cell, thereby providing insights into the effects of these defects on the material's overall behavior using VESTA software.
The results show significant changes in the electronic structure, bandgap and density of states due to defect introduction.

Introductions:

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.



Title: ZrC

Lattice type F
Space group name F m -3 m
Space group number 225
Setting number 1

Lattice parameters

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

Unit-cell volume = 107.850192 Å^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

Number of polygons and unique vertices on isosurface = 0 (0)
27 atoms, 0 bonds, 0 polyhedra; CPU time = 2 m

Super Cell:

A super-cell is a repeating unit cell of a crystal that contains multiple primitive cells. OR A super-cell is a larger unit cell that describes the same crystal as a smaller unit cell, called the unit cell. In some cases, the primitive cells of a crystal can be perturbed to create a supercell that becomes the new primitive cell. The supercell approximation can be used to imply periodicity in disordered systems while preserving local disordered properties.

Transformation into super cell

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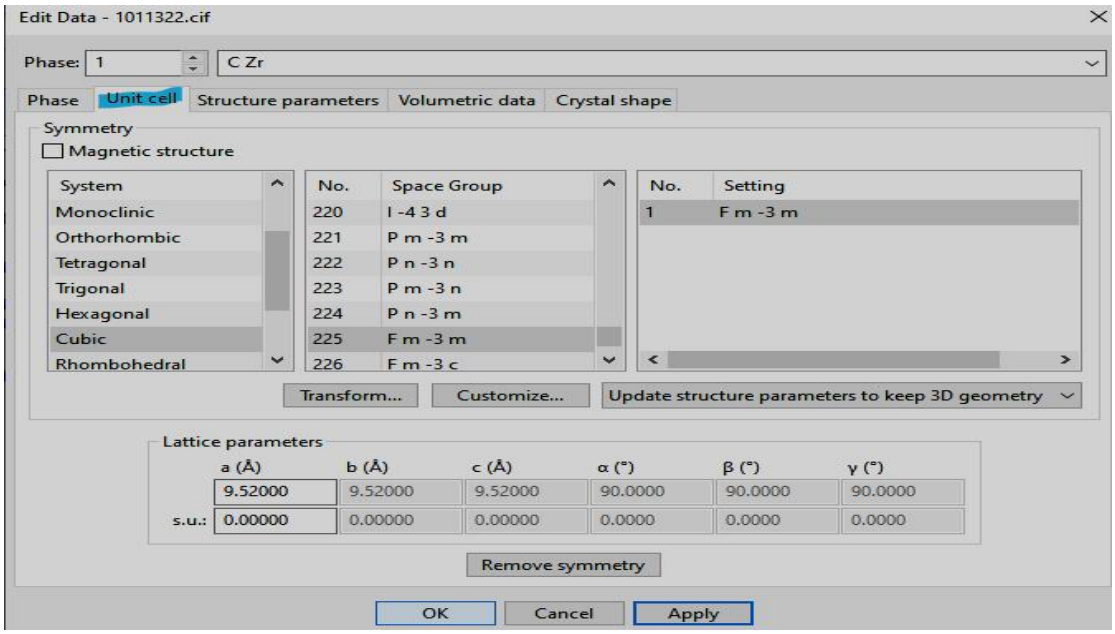
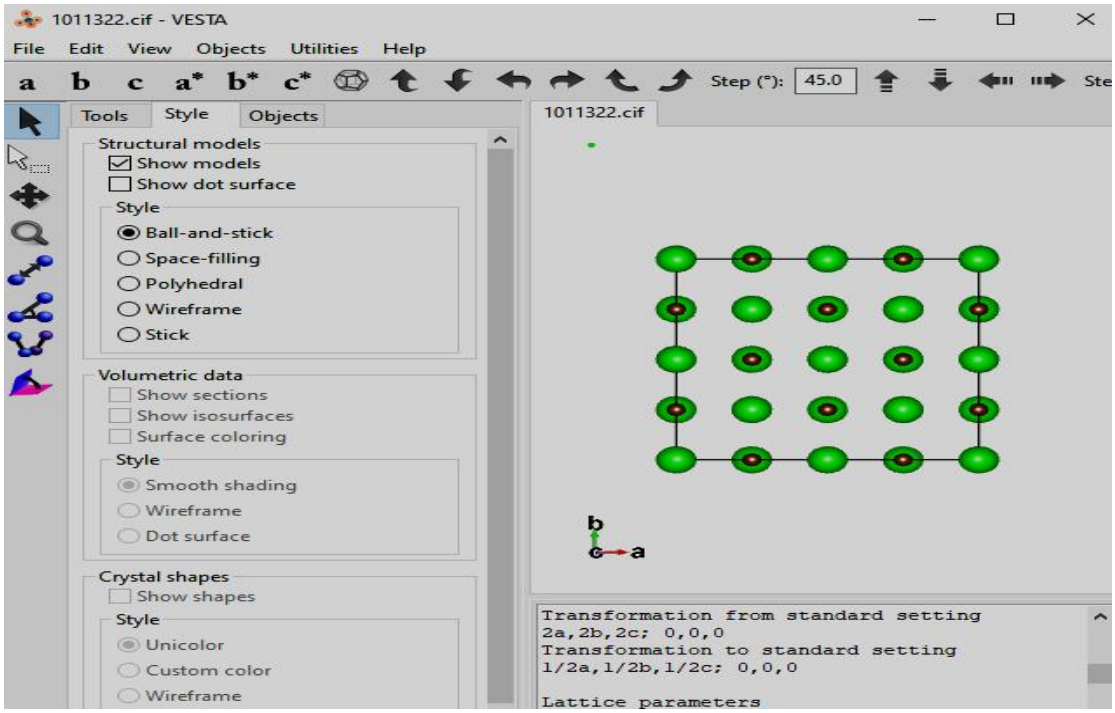




Lattice type F
Space group name F m -3 m
Space group number 225
Setting number 1
Transformation from standard setting 2a,2b,2c; 0,0,0
Transformation to standard setting 1/2a,1/2b,1/2c; 0,0,0

Lattice parameters

a	b	c	alpha	beta	gamma
9.52000	9.52000	9.52000	90.0000	90.0000	90.0000

Unit-cell volume = 862.801532 Å^3
Number of polygons and unique vertices on iso surface = 0 (0)
125 atoms, 0 bonds, 0 polyhedral; CPU time = 4 ms

Point defects:

A point defect occurs when one or more atoms of a crystalline solid leave their original lattice site and/or foreign atoms occupy the interstitial position of the crystal.

There are 3 types of point defects:

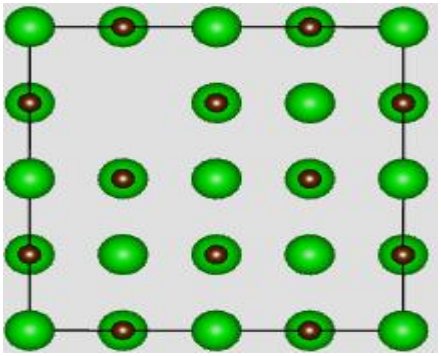
1. **Stoichiometric defect**
2. **Schottky defect**
3. **Frenkel defect**

1. Stichiometric defects

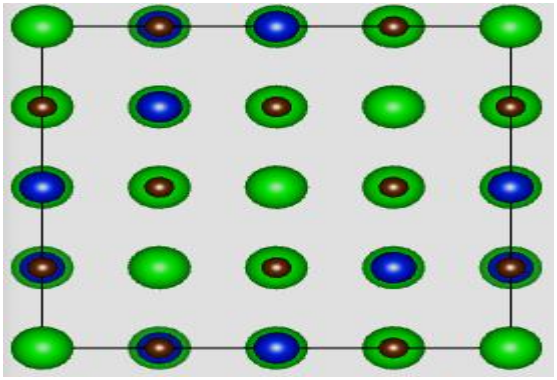
In this kind of point defect, the ratio of positive and negative ions (Stoichiometric) and electrical neutrality of a solid is not disturbed. Sometimes it is also known as intrinsic or thermodynamic defects.

Fundamentally, they are of two types:

- **Vacancy defect:** When an atom is not present at their lattice sites, then that lattice site is vacant and it creates a vacancy defect. Due to this, the density of a substance decreases.

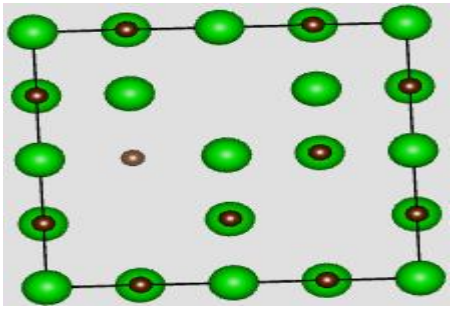


- **Substitutional defect:** It is a defect in which an atom or molecule occupies the intermolecular spaces in crystals. In this defect, the density of the substance increases.



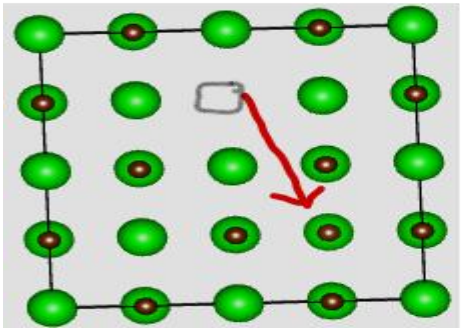
2. Schottky defect:

Schottky defects involve the absence of both cations and anions from their regular lattice sites, resulting in lattice vacancies.



3.Frankel defect:

Frenkel defects, on the other hand, occur when a cation moves to an interstitial site, leaving behind a vacancy at its original lattice position.



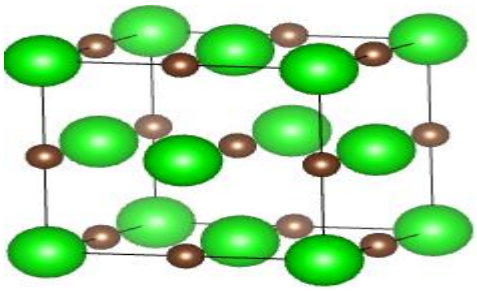
Equipment or Accessories:

- Compute or laptop with VESTA software installed
- Crystallographic data files (CIF)
  Zirconium Carbide (ZrC)

Experimental Design:

- I launch the VESTA software and open a CIF file of a solid material Zirconium Carbide (ZrC).
- Then I, analyze the crystal structure e.g lattice type, lattice parameters, space group etc.
- Then I made, a supercell by using VESTA tools:
- Go to Edit menu
- Then click on Edit data in which I choose unit cell tool then click on Transform ,after that 1 change their diagonal position, click on apply. Finally a supercell is formed.
- After the formation of supercell, I create defects in that structure, by the addition of an impurity of Silicon element.
- Then I visualize all crystal defects e.g Schotkky defect, Frenkel defect and further their types one by one.
- Also, observed the powder diffraction pattern of supercell, and study the variation of intensity verses diffraction angle 2ɵ. in the form of table.
- Then I found the output.

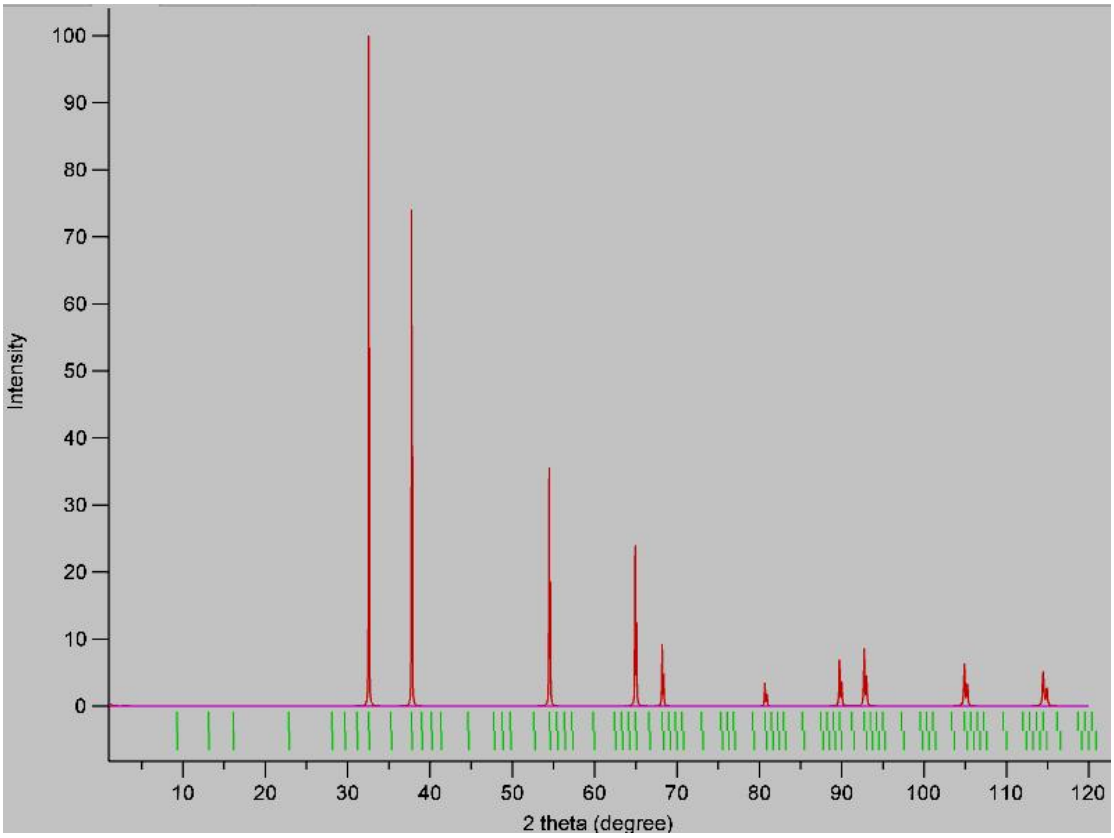
Structure:



Observation:

h	k	l	intensity	Diffraction angle(2ɵ)	Wavelength(λ)
2	2	2	100.00	32.5553	1
4	0	0	79.5864	37.7681	1
4	4	0	52.2742	54.4796	1
2	2	2	49.7441	32.6364	2

Analysis:



Output:

attice type F
Space group name F m -3 m
Space group number 225
Setting number 1
Lattice parameters:

Bond lengths:

a	b	c
4.76000	4.7600	4.7600

Bond angles

alpha	beta	gamma
90.0000	90.0000	90.0000

Unit-cell volume = 107.850192 Å^3
Number of polygons and unique vertices on isosurface = 0 (0)
27 atoms, 0 bonds, 0 polyhedra; CPU time = 7 ms

125 atoms, 0 bonds, 0 polyhedra; CPU time = 11 ms

125 atoms, 0 bonds, 0 polyhedra; CPU time = 9 ms

For Energy calculation:
Radius of an ionic sphere: 2.00 Å
Reciprocal-space range: 2.00 Å**(-1)
Number of symmetry operations: 96
Number of atoms in the asymmetric unit: 16
Inversion center at the origin: 1

Lattice parameters: 9.5200 9.5200 9.5200 90.000 90.000 90.000

Electrostatic energy per asymmetric unit
-1.957717 e**2/Å = -28.19045 eV = -2.719964 MJ/mol

Conclusion:

This experiment successfully demonstrated the construction and simulation of point defects in solids using the supercell approach. Also investigate the interaction between vacancy defects and other impurities. This results provided valuable insights into the effects of defects on the electronic and structural properties.