Crystal Structure Analysis: Unit Cells, Miller Indices, and X-Ray Diffraction Patterns

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Abstract

This technical report presents a comprehensive analysis of crystal structures in materials science. We examine unit cell geometry, Miller index notation, interplanar spacing calculations, and X-ray diffraction pattern simulation. Computational analysis using Python demonstrates structure factor calculations and powder diffraction profiles for common crystal systems.

1 Introduction

Crystallography forms the foundation for understanding material properties. The periodic arrangement of atoms determines mechanical, electrical, and optical characteristics.

Definition 1.1 (Miller Indices)**.** *Miller indices* (hkl) *describe the orientation of crystal planes through the reciprocals of the intercepts on crystallographic axes, reduced to the smallest integers.*

2 Unit Cell Geometry

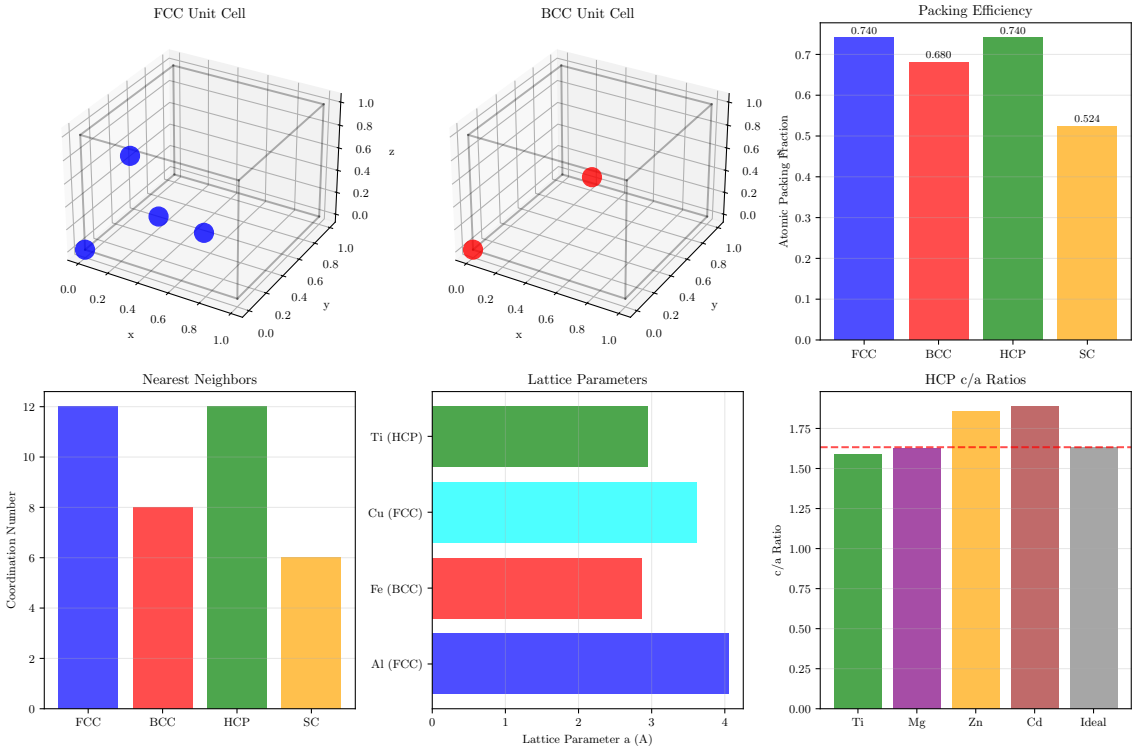

Figure 1: Unit cell structures and crystallographic parameters for common crystal systems.

Table 1: Crystal Structure Properties

Structure	APF	CN	Atoms/Cell	Examples
FCC	0.740	12	4	Al, Cu, Au
BCC	0.680	8	2	Fe, W, Cr
HCP	0.740	12	2	Ti, Mg, Zn
SC	0.524	6	1	Po

3 Miller Indices and Interplanar Spacing

Theorem 3.1 (Interplanar Spacing). *For a cubic crystal system, the spacing between* (hkl) *planes is:*

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \tag{1}$$

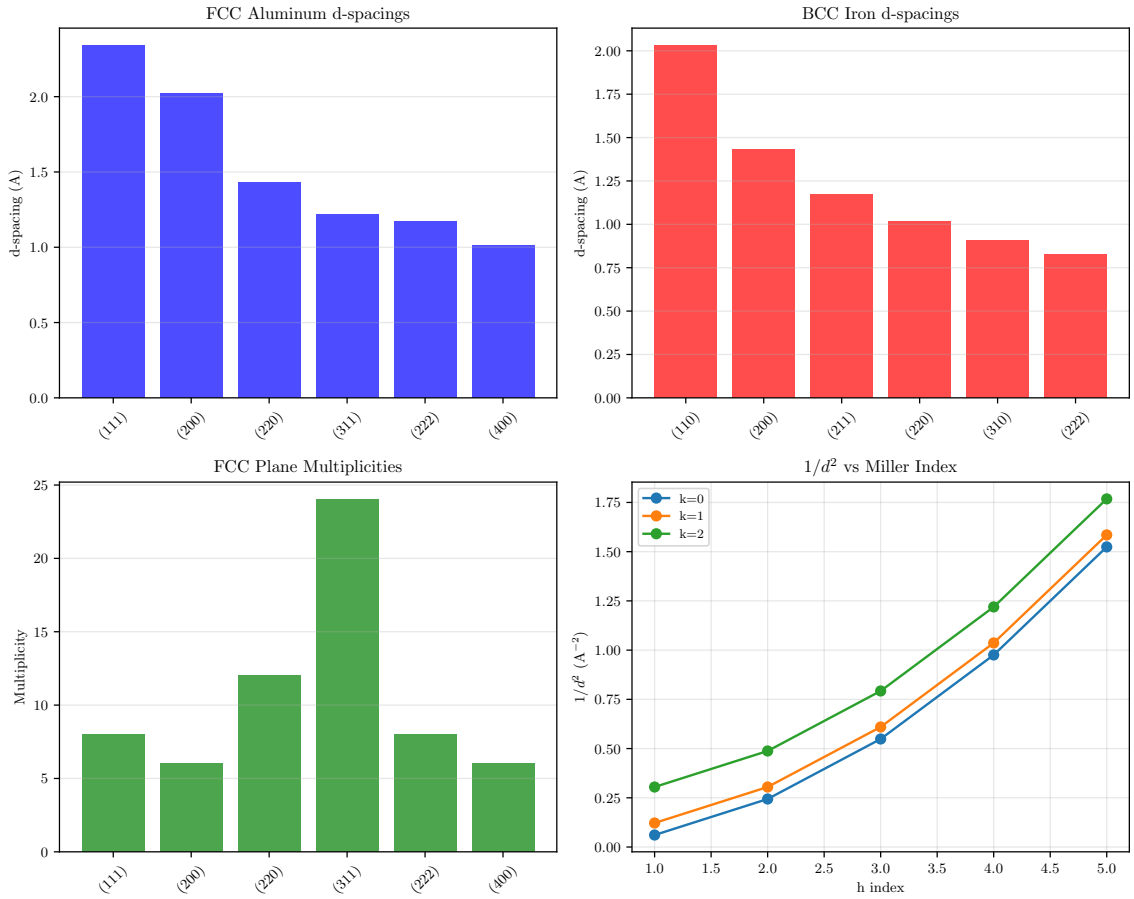

Figure 2: Interplanar spacing and multiplicity factors for FCC and BCC structures.

4 X-Ray Diffraction Simulation

Definition 4.1 (Bragg's Law). *Constructive interference occurs when:*

$$n\lambda = 2d_{hkl} \sin\theta \tag{2}$$

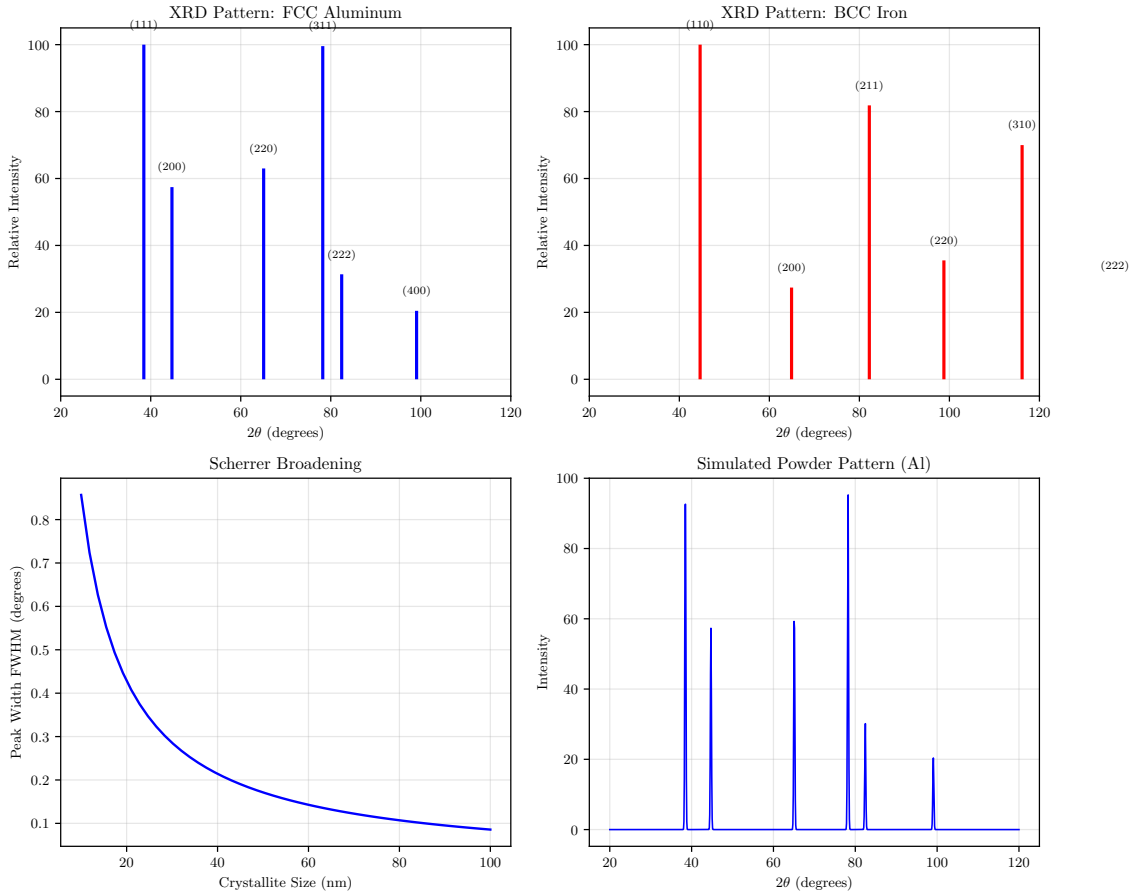

Figure 3: X-ray diffraction patterns and peak characteristics for FCC and BCC metals.

5 Structure Factor Analysis

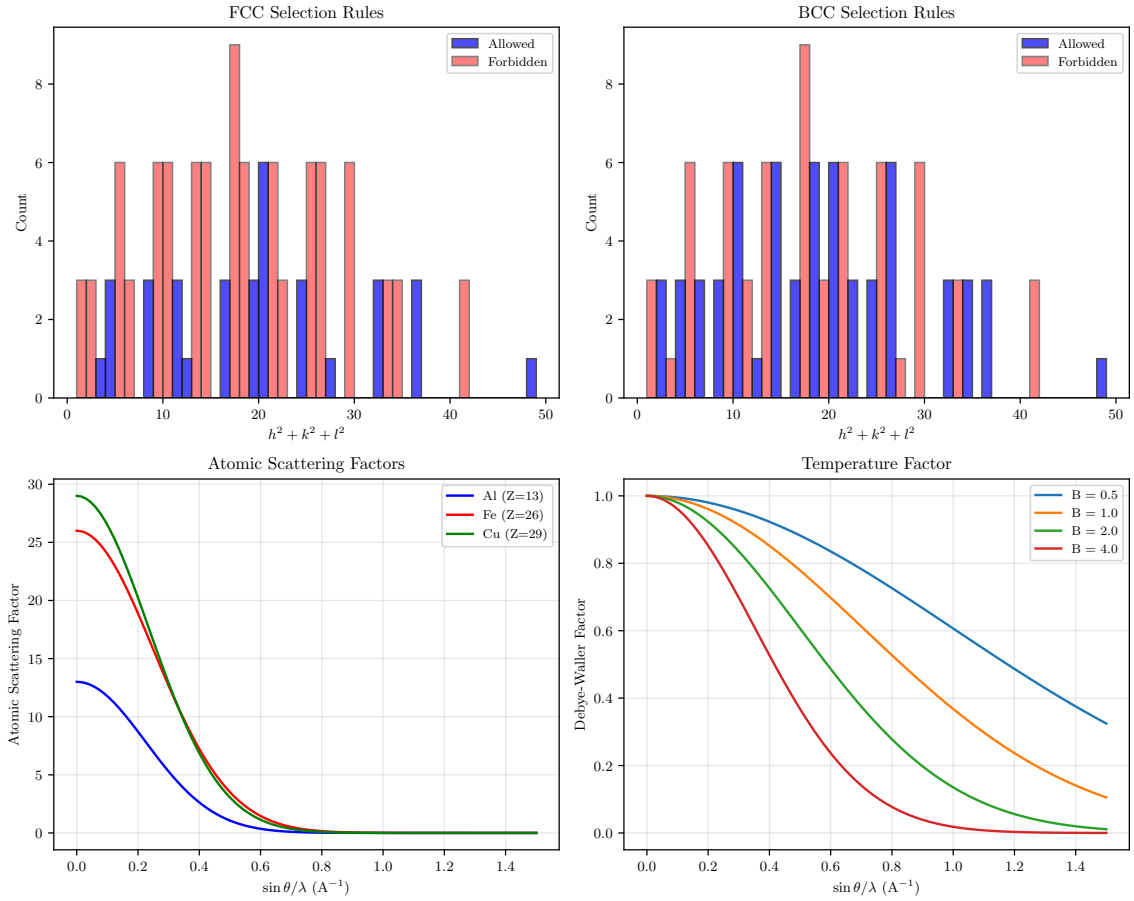

Figure 4: Structure factor analysis: selection rules and scattering factors.

6 Lattice Strain and Defect Analysis

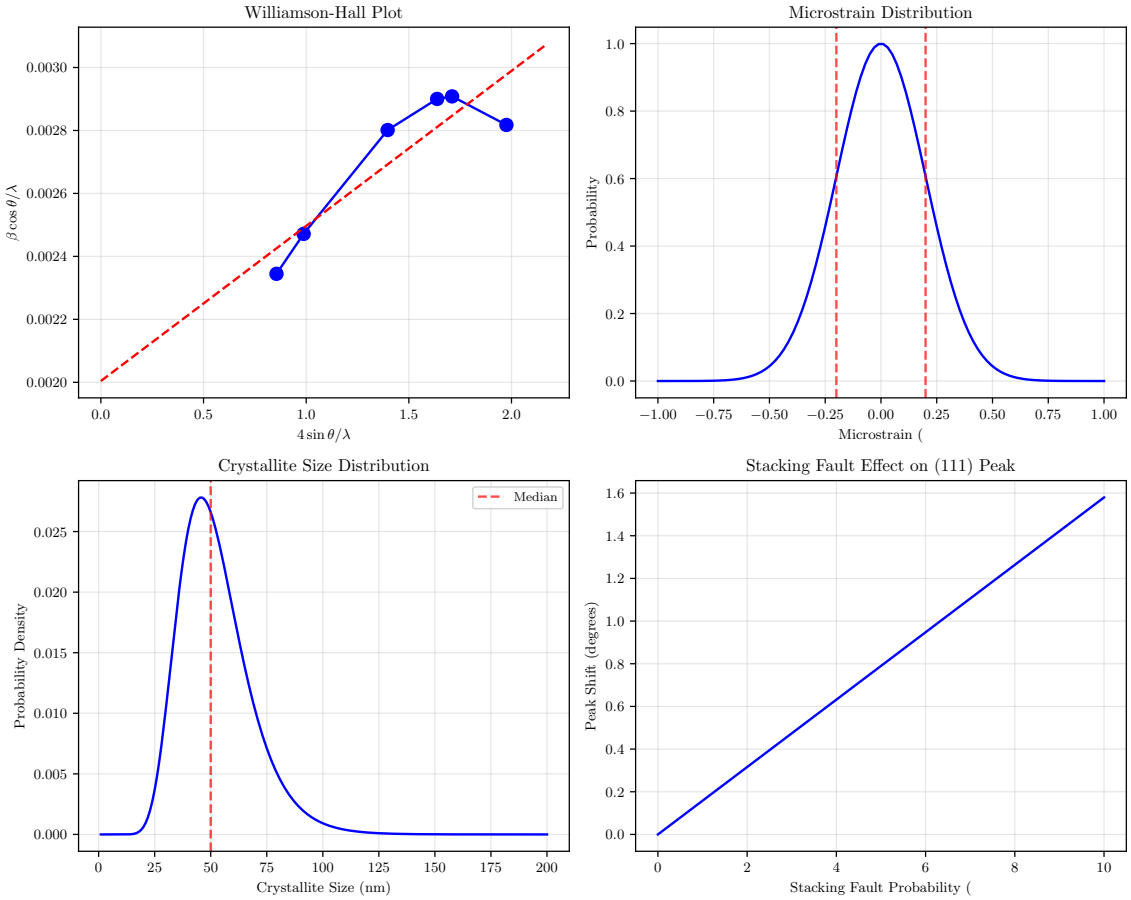

Figure 5: Microstructural analysis: Williamson-Hall plot and defect characterization.

Table 2: Microstructural Parameters

Parameter	**Value**	**Unit**
Crystallite Size	50	nm
Microstrain	0.20	%
Dislocation Density	1.71e+03	m^{-2}

7 Conclusions

This analysis of crystal structures demonstrated:

1. **Unit Cell Geometry**: FCC has the highest packing efficiency (APF = 0.740) with coordination number 12.

2. **Miller Indices**: Interplanar spacing follows $d_{hkl} = a/\sqrt{h^2 + k^2 + l^2}$ for cubic systems, with the (111) plane having the largest d-spacing in FCC.

3. **XRD Patterns**: Selection rules determine allowed reflections (all odd or all even for FCC, $h + k + l$ = even for BCC).

4. **Structure Factors**: Systematic absences provide fingerprints for crystal structure identification.

5. **Defect Analysis**: Williamson-Hall analysis separates size ($D = 50$ nm) and strain ($\epsilon = 0.20\%$) contributions to peak broadening.