

Appendix-I: Simulated spot electron diffraction patterns

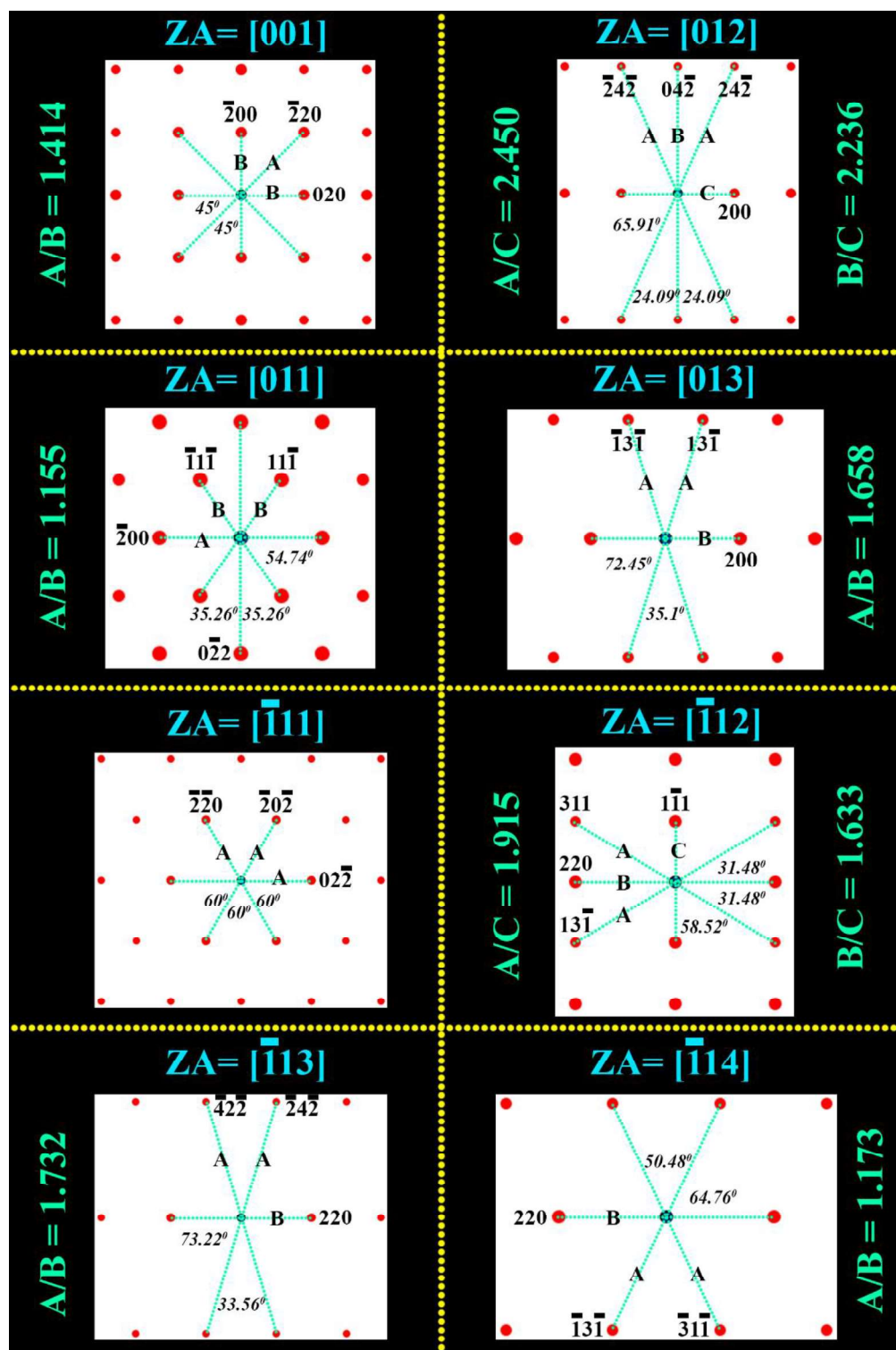


Figure A.1: Single-crystal spot electron diffraction patterns from several zone axis of a FCC structure ($u^2+v^2+w^2 < 22$). The patterns have been simulated with the help of JEMS software. The respective zone axis directions are marked as “ZA” on top of each pattern. The ratio of the principal vectors along with the interplanar angles are marked in the respective patterns.

Appendix-II: Python code for XRD pattern simulation

Excerpt from the python code for simulation of x-ray diffraction (XRD) patterns:

```
"cell_type": "code",
"execution_count": 226,
"id": "abc88470-a468-4a2e-be0e-482a5c05390e",
"metadata": {},
"outputs": [],
"source": [
"material = 'w-Ti'\n",
"lattice_type='hexagonal'\n",
"wavelength=1.54\n",
"a=4.6\n",
"b=4.6\n",
"c=2.82\n",
"\n",
"alpha= 90\n",
"beta= 90\n",
"gamma=90\n",
"alpha_rad = math.radians(alpha)\n",
"beta_rad = math.radians(beta)\n",
"gamma_rad = math.radians(gamma)\n",
"lattice={}\n",
"\n",
"motifs = {\n",
" #\"Al\": np.array([[0.0, 0.0, 0.0],[0.5,0.5,0.0],[0.5,0.0,0.5],[0.0,0.5,0.5]]),\n",
" #\"Mn\": np.array([[0.5, 0.5, 0.5],[0.0,0.0,0.5],[0.0,0.5,0.0],[0.5,0.0,0.0]]),\n",
" #\"Cu\":
np.array([[1/4, 1/4, 1/4],[3/4,3/4,3/4],[3/4,3/4,1/4],[3/4,1/4,3/4],[1/4,3/4,3/4],[1/4,1/4,3/4
],[1/4,3/4,1/4],[3/4,1/4,1/4]])\n",
```

```

" #\"Cu\": np.array([[0.5,0.0,0.5],[0.0,0.5,0.5]])\n",
"
" #\"Si\": np.array([[0.0, 0.0,
0.0],[0.5,0.5,0.0],[0.5,0.0,0.5],[0.0,0.5,0.5],[1/4,1/4,1/4],[3/4,3/4,1/4],[3/4,1/4,3/4],[1/4,
3/4,3/4]]),\n",
" #\"As\": np.array([[1/3, 2/3, 1/4],[2/3,1/3,3/4]])\n",
" #\"Ti\": np.array([[0.0, 0.0, 0.0], [1/3, 2/3, 1/2],[2/3,1/3,1/2]])\n",
" #\"Sn\": np.array([[0.0,0.0,0.0],[0.5, 0.5, 0.5],[0.0,1/2,1/4],[1/2,0.0,3/4]])\n",
"
"}\n",
"\n",
"#motifs = np.array([[0.0, 0.0, 0.0], [0.0, 0.5, 0.5],[0.5, 0.0, 0.5],[0.5, 0.5, 0.0]])\n",
"#motifs = np.array([[0.0, 0.0, 0.0], [0.5, 0.5, 0.5]])\n",
"#motifs = np.array([[0.0, 0.0, 0.0], [2/3, 1/3, 1/2]])\n",
"#motifs = np.array([[0.0, 0.0, 0.0]])\n",
"\n",
"peak_positions = []\n",
"peak_intensity=[]\n",
"df=pd.read_csv(\"atomic_scattering_factor.csv\")\n",
"df_raw = pd.read_excel(\"lorentz_polarization_factor.xlsx\", header=0)"
]
},
{
"cell_type": "code",
"execution_count": 228,
"id": "b8079682-aa88-4ae7-bbcb-7ec852f5dcfb",
"metadata": {},
"outputs": [
{
"name": "stdout",
"output_type": "stream",
"text": [

```

```

"rounded 0.4\n",
"10.9\n"
]
}
],
"source": [
"def find_fo(h,k,l,element):\n",
"    s11 = b**2 * c**2 * math.sin(alpha_rad)**2\n",
"    s22= a**2 * c**2 * math.sin(beta_rad)**2\n",
"    s33= a**2 * b**2 * math.sin(gamma_rad)**2\n",
"    s12 = a * b * c**2 * (math.cos(alpha_rad) * math.cos(beta_rad) -
math.cos(gamma_rad))\n",
"    s23 = c * b * a**2 * (math.cos(beta_rad) * math.cos(gamma_rad) -
math.cos(alpha_rad))\n",
"    s13 = a * c * b**2 * (math.cos(gamma_rad) * math.cos(alpha_rad) -
math.cos(beta_rad))\n",
"    v = a * b * c * math.sqrt((1 - math.cos(alpha_rad)**2 - math.cos(beta_rad)**2 -
math.cos(gamma_rad)**2 + 2 * math.cos(alpha_rad) * math.cos(beta_rad) *
math.cos(gamma_rad)))\n",
"    \n",
"\n",
"    numerator = s11 * h**2 + s22 * k**2 + s33 * l**2 + 2 * s12 * h * k + 2 * s23 * k *
l + 2 * s13 * l * h\n",
"    d = v / math.sqrt(numerator)\n",
"    d=round(d,2)\n",
"    theta = np.arcsin(wavelength / (2 * d))\n",
"    theta=round(theta,2)\n",
"    position= round(np.degrees(2*theta),2)\n",
"\n",
"    temp= (math.sin(math.radians(position/2)))/wavelength\n",
"    rounded_temp = round(temp, 1)\n",
"    value=1\n",

```

```
" print(\\"rounded\\",rounded_temp)\n",  
" try:\n",  
"     value = df.loc[df['Element'] == element, str(rounded_temp)].values[0]\n",  
" except KeyError:\n",  
"     value=1\n",  
" return value\n",  
"print(find_fo(0,0,2,'Ti'))\n"  
]  
}
```

LIST OF PUBLICATIONS

1. *Saptarshi Mukherjee*, N.K. Mukhopadhyay, Joysurya Basu, Composition modulation, strain minimization and oriented growth of phases in equimolar (CaCoFeMgNi) multicomponent oxide, *Acta Mater.*, 2025, 285, 120621 (12 pages)
2. *Saptarshi Mukherjee*, N.K. Mukhopadhyay, Joysurya Basu, Structural modulation and oriented growth of spinel and rocksalt phases in equimolar (Co(Cr/Mg)FeMnNi) multicomponent oxide and its derivatives, *J. Am. Ceram. Soc.*, 2025, e20619 (15 pages)
3. *Saptarshi Mukherjee*, Sandip Bysakh, N.K. Mukhopadhyay, Joysurya Basu, Local composition modulation and oriented inter-growth induced strain minimization in entropy stabilized (CoCuMgNiZn)-oxide [Communicated]
4. *Saptarshi Mukherjee*, Shivank Shukla, Chanchal Ghosh, N.K. Mukhopadhyay, Joysurya Basu, Phase Stability and microstructural evolution in vanadium-titanium alloys with oxygen dissolution and varying titanium-content, *Microscopy and Microanalysis*, 2020, Vol. 26 (S2), 2086-2088
5. *Saptarshi Mukherjee*, Rajdeep Chatterjee, Urwashi Gupta, B. Mukherjee N.K. Mukhopadhyay, Joysurya Basu, Structure-activity relationship for electrocatalysis in rocksalt and spinel based multicomponent oxides and its derivatives [To be communicated]
6. *Saptarshi Mukherjee*, N.K. Mukhopadhyay, Joysurya Basu, Revisiting the aspects of phase formation, microstructural evolution and its stability in rocksalt and spinel forming high entropy oxides [To be communicated]

LIST OF CONFERENCE PRESENTATIONS

1. Oral presentation at the National Student's Seminar on Metallurgy and Materials Science (**BTTD-2024**), by IIM (Jamshedpur chapter) in association with CSIR-NML and Tata Steel Ltd. during June 19-21st, 2024.
Recipient of Best Oral Presentation Award
2. Oral and poster presentation at the International Conference on Electron Microscopy (**EMSI-2024**), by IIT Bombay during May 16-18th, 2024.
Recipient of Best Poster Presentation Award
3. Oral presentation at the National Symposium of Research Scholars (**NSRS-2024**) on Metallurgy and Materials, by IIT Kanpur during March 9-10th, 2024.
Recipient of Best Oral Presentation Award
4. Poster presentation at the 20th International Microscopy Congress (**IMC20**) in Busan, Republic of Korea during September 10-15th, 2023.
Recipient of Travel Bursary Awards from RMS, UK and EMSI, India
5. Poster presentation at the International Conference on Electron Microscopy (**EMSI-2023**) in Delhi, during February 8-10th, 2023.
6. Oral presentation at Microscopy and Microanalysis (**M&M-2020**), Milwaukee during August 3-7th, 2020.
7. Oral presentation at the Early Career European Microscopy Congress (**EMC-2020**), Copenhagen during November 24-26th, 2020.
8. Poster presentation at the 12th Asia-Pacific Microscopy Conference (**APMC-2020**), Hyderabad during February 3-7th, 2020.