

Numerical Calculations of the Structure Factor of GaAs

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In this section we numerically calculate the structure factor for GaAs. The structure factor is defined as

$$M_p(\mathbf{K}) = \sum_{j=1}^n f^{(j)}(\mathbf{K}) e^{-i\mathbf{K} \cdot \mathbf{d}_j}$$

where \mathbf{K} is a vector in the reciprocal lattice, $f^{(j)}$ is the atomic form factor of atom j , d_j is the position of an atom in the basis, and the sum ranges over all atoms in the basis.

We used a cubic lattice with a 8 atom basis for our calculations. We evaluated the structure factor for all $|\mathbf{K}| \leq 4\frac{2\pi}{a}$ in the reciprocal lattice where a is the lattice spacing of the direct lattice. The Matlab code we used to do these calculations is contained in Appendix A.

The following table lists the magnitude of the structure factor for the desired \mathbf{K} in the reciprocal lattice. Since the structure factor only depends on the magnitude of \mathbf{K} , redundant permutations are not listed in the table. For example, (001) is listed but (010) is not.

(hkl)	$ \mathbf{K} $
(000)	255.8356
(001)	0
(002)	5.5778
(003)	0
(004)	163.0762
(011)	0
(012)	0
(013)	0
(022)	190.0949
(023)	0
(111)	155.0049
(112)	0
(113)	126.2948
(122)	0
(123)	0
(222)	5.0043
(400)	163.0762

A Matlab Code

This appendix contains the matlab code used to calculate the structure factor. The code consists of `aff.m` and `structure.m`. `aff.m` is a function that calculates structure factors for a given Miller index in the reciprocal lattice. `structure.m` is a sloppy script that calculates the structure factor for all $\mathbf{K} \leq 4\frac{2\pi}{a}$.

A.1 `aff.m`

```
function [Gallium, Arsenic]=aff(h,k,l)
% Takes a set of Miller indices [hkl] and calculates the atomic
% form factors for Ga and As.

global Gallium Arsenic

% Lattice constant and Sin Theta over Lambda
a = 5.6419; %given in Angstroms
stl = sqrt(h^2+k^2+l^2)/(2*a);

% Gallium
a1 = 15.2354;
b1 = 3.06690;
a2 = 6.7006;
b2 = 0.2412;
a3 = 4.35910;
```

```

b3 = 10.7805;
a4 = 2.96230;
b4 = 61.4135;
c = 1.71890;
f = a1*exp(-b1*stl*stl) + a2*exp(-b2*stl*stl) + a3*exp(-b3*stl*stl)...
  + a4*exp(-b4*stl*stl) + c;
Gallium = f;

% Arsenic
a1 = 16.6723;
b1 = 2.63450;
a2 = 6.07010;
b2 = 0.2647;
a3 = 3.4313;
b3 = 12.9479;
a4 = 4.2779;
b4 = 47.7972;
c = 2.531;
f2 = a1*exp(-b1*stl*stl) + a2*exp(-b2*stl*stl) + a3*exp(-b3*stl*stl)...
  + a4*exp(-b4*stl*stl) + c;
Arsenic = f2;

```

A.2 structure.m

% This function calculates the structure factor for various Miller indices
% in the reciprocal lattice.

```

global Arsenic Gallium
a = 5.6419; %given in Angstroms

for h = 0:4
  for k = 0:4
    for l = 0:4
      if sqrt(h^2 + k^2 + l^2) <= 4
        K = 2*pi/a * [h; k; l];
        aff(h,k,l);
        [h; k; l]
        sum = Gallium * exp(-i * dot(K, [0;0;0]));
        sum = sum + Gallium * exp(-i * dot(K, [a/2;a/2;0]));
        sum = sum + Gallium * exp(-i * dot(K, [0;a/2;a/2]));
        sum = sum + Gallium * exp(-i * dot(K, [a/2;0;a/2]));
        sum = sum + Arsenic * exp(-i * dot(K, [a/4;a/4;a/4]));
        sum = sum + Arsenic * exp(-i * dot(K, [3*a/4;a/4;3*a/4]));
        sum = sum + Arsenic * exp(-i * dot(K, [3*a/4;3*a/4;a/4]));
        sum = sum + Arsenic * exp(-i * dot(K, [a/4;3*a/4;3*a/4]));
        abs(sum)
      end
    end
  end
end

```

end
end
end
end