

WFU Physics Colloquium

TITLE: Crystal Structure, Electronic Structure and Physicochemical Characterization of Multi-Cation Diamond-Like Semiconductors

SPEAKER: Professor Jennifer Aitken,
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TIME: Wednesday April 9, 2014 at 4:00 PM

PLACE: Room 101 Olin Physical Laboratory

Refreshments will be served at 3:30 PM in the Olin Lounge. All interested persons are cordially invited to attend.

ABSTRACT

Diamond-like semiconductors (DLs) possess crystal structures that can be considered as derivatives of cubic or hexagonal diamond. DLs are one of the few classes of solid-state compounds, for which all chemical compositions can be calculated and a set of possible structures postulated. The use of the many elements that can adopt tetrahedral coordination leads to a multitude of possible compounds, and solid solutions thereof, that can be exploited for physical property tuning. The compositional flexibility and structural simplicity of these materials provides an avenue to develop an intimate understanding of composition-property and structure-property correlations. This seminar will cover our recent progress toward this goal made during our search for DLs with applications in non-linear optics and thermoelectrics, and as lithium ion conductors.

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Generation of X-rays in a Coolidge tube
<https://www.orau.org/ptp/collection/xraytubescoolidge/coolidgeinformation.htm>

The diagram illustrates the components of a Coolidge tube. An electron beam is directed from a cathode towards a tungsten anode. The anode is mounted on an anode arm, and the cathode is on a cathode arm. The resulting X-ray beam is emitted from the point of impact between the electron beam and the anode.

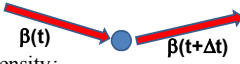
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<http://www.ndt-ed.org/EducationResources/CommunityCollege/Radiography/Physics/xrays.htm>

The graph shows the X-ray spectrum from a molybdenum target. The y-axis represents Photon Counts, ranging from 0.0e+000 to 2.0e+004. The x-axis represents Energy in keV, ranging from 0 to 150. The spectrum features two sharp characteristic peaks at approximately 20 keV and 23 keV, and a continuous spectrum that starts at about 20 keV and extends to higher energies.

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Radiation during collisions



Intensity:

$$\frac{d^2 I}{d\omega d\Omega} = \frac{q^2}{4\pi^2 c} \left| \int dt e^{i\omega(t-\hat{r}\cdot\mathbf{R}_q(r)/c)} \frac{d}{dt} \left[\frac{\hat{r} \times (\hat{r} \times \boldsymbol{\beta})}{1 - \hat{r} \cdot \boldsymbol{\beta}} \right] \right|^2$$

Note that $\hat{r} \times (\hat{r} \times \boldsymbol{\beta}) = (\boldsymbol{\epsilon}_1 \cdot \boldsymbol{\beta})\boldsymbol{\epsilon}_1 + (\boldsymbol{\epsilon}_2 \cdot \boldsymbol{\beta})\boldsymbol{\epsilon}_2$
 For a collision of duration τ emitting radiation with polarization $\boldsymbol{\epsilon}$ and frequency $\omega \rightarrow 0$:

$$\frac{d^2 I}{d\omega d\Omega} = \frac{q^2}{4\pi^2 c} \left| \boldsymbol{\epsilon} \cdot \left(\frac{\boldsymbol{\beta}(t+\tau)}{1 - \hat{r} \cdot \boldsymbol{\beta}(t+\tau)} - \frac{\boldsymbol{\beta}(t)}{1 - \hat{r} \cdot \boldsymbol{\beta}(t)} \right) \right|^2$$

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Radiation during collisions -- continued

For a collision of duration τ emitting radiation with polarization $\boldsymbol{\epsilon}$ and frequency $\omega \rightarrow 0$:

$$\frac{d^2 I}{d\omega d\Omega} = \frac{q^2}{4\pi^2 c} \left| \boldsymbol{\epsilon} \cdot \left(\frac{\boldsymbol{\beta}(t+\tau)}{1 - \hat{r} \cdot \boldsymbol{\beta}(t+\tau)} - \frac{\boldsymbol{\beta}(t)}{1 - \hat{r} \cdot \boldsymbol{\beta}(t)} \right) \right|^2$$

Non - relativistic limit:

$$\frac{d^2 I}{d\omega d\Omega} = \frac{q^2}{4\pi^2 c} \left| \boldsymbol{\epsilon} \cdot (\Delta\boldsymbol{\beta}) \right|^2 \quad \Delta\boldsymbol{\beta} \equiv \boldsymbol{\beta}(t+\tau) - \boldsymbol{\beta}(t)$$

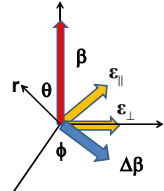
Relativistic collision with small $|\Delta\boldsymbol{\beta}|$:

$$\frac{d^2 I}{d\omega d\Omega} = \frac{q^2}{4\pi^2 c} \left| \boldsymbol{\epsilon} \cdot \left(\frac{\Delta\boldsymbol{\beta} + \hat{r} \times (\boldsymbol{\beta} \times \Delta\boldsymbol{\beta})}{(1 - \hat{r} \cdot \boldsymbol{\beta})^2} \right) \right|^2$$

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Radiation during collisions -- continued

Relativistic collision with small $|\Delta\boldsymbol{\beta}|$:



$$\frac{d^2 I}{d\omega d\Omega} = \frac{q^2}{4\pi^2 c} \left| \boldsymbol{\epsilon} \cdot \left(\frac{\Delta\boldsymbol{\beta} + \hat{r} \times (\boldsymbol{\beta} \times \Delta\boldsymbol{\beta})}{(1 - \hat{r} \cdot \boldsymbol{\beta})^2} \right) \right|^2$$

Expressions (averaging over ϕ) for \parallel or \perp polarization:

$$\frac{d^2 I_{\parallel}}{d\omega d\Omega} = \frac{q^2}{8\pi^2 c} |\Delta\boldsymbol{\beta}|^2 \frac{(\beta - \cos\theta)^2}{(1 - \beta \cos\theta)^4} \quad \text{polarization in } r \text{ and } \boldsymbol{\beta} \text{ plane}$$

$$\frac{d^2 I_{\perp}}{d\omega d\Omega} = \frac{q^2}{8\pi^2 c} |\Delta\boldsymbol{\beta}|^2 \frac{1}{(1 - \beta \cos\theta)^2} \quad \text{polarization perpendicular to } r \text{ and } \boldsymbol{\beta} \text{ plane}$$

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Radiation during collisions -- continued

Relativistic collision at low ω and with small $|\Delta\beta|$ and $\Delta\beta$ perpendicular to plane of \hat{r} and β , as a function of θ where $\hat{r} \cdot \beta = \beta \cos \theta$;
 Integrating over solid angle:

$$\frac{dI}{d\omega} = \int d\Omega \left(\frac{d^2 I_{\parallel}}{d\omega d\Omega} + \frac{d^2 I_{\perp}}{d\omega d\Omega} \right) = \frac{2}{3\pi} \frac{q^2}{c} \gamma^2 |\Delta\beta|^2$$

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Estimation of $\Delta\beta$

Momentum transfer:
 $Q \equiv |\mathbf{p}(t + \tau) - \mathbf{p}(t)| \approx \gamma M c^2 |\Delta\beta|$
 mass of particle having charge q

$$\frac{dI}{d\omega} = \frac{2}{3\pi} \frac{q^2}{c} \gamma^2 |\Delta\beta|^2 \approx \frac{2}{3\pi} \frac{q^2}{M^2 c^3} Q^2$$

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Estimation of $\Delta\beta$ -- for the case of Rutherford scattering

Assume that target nucleus (charge Ze) has mass $\gg M$;
 Rutherford scattering cross-section:

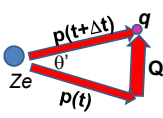
$$\frac{d\sigma}{d\Omega} = \left(\frac{2Ze q}{pv} \right)^2 \frac{1}{(2 \sin(\theta/2))^4}$$

 Assuming elastic scattering:

$$Q^2 = (2p \sin(\theta/2))^2 = 2p^2 (1 - \cos \theta)$$

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Case of Rutherford scattering -- continued



Rutherford scattering cross-section:

$$\frac{d\sigma}{d\Omega} = \left(\frac{2Ze q}{pv}\right)^2 \frac{1}{(2\sin(\theta'/2))^4}$$

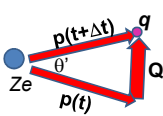
$$\frac{d\sigma}{dQ} = \int d\phi' \frac{d\sigma}{d\Omega} \frac{d\Omega}{dQ}$$

$$Q^2 = (2p \sin(\theta'/2))^2 = 2p^2(1 - \cos \theta')$$

$$\Rightarrow \frac{d\sigma}{dQ} = 8\pi \left(\frac{Ze q}{\beta c}\right)^2 \frac{1}{Q^3}$$

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Case of Rutherford scattering -- continued



Differential radiation cross section:

$$\frac{d^2\chi}{d\omega dQ} = \frac{dI}{d\omega} \frac{d\sigma}{dQ} = \left(\frac{2}{3\pi} \frac{q^2}{M^2 c^3} Q^2\right) \left(8\pi \left(\frac{Ze q}{\beta c}\right)^2 \frac{1}{Q^3}\right)$$

$$= \frac{16}{3} \frac{(Ze)^2}{c} \left(\frac{q^2}{Mc^2}\right)^2 \frac{1}{\beta^2} \frac{1}{Q}$$

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Differential radiation cross section -- continued

Integrating over momentum transfer

$$\frac{d\chi}{d\omega} = \int_{Q_{\min}}^{Q_{\max}} dQ \frac{d^2\chi}{d\omega dQ} = \frac{16}{3} \frac{(Ze)^2}{c} \left(\frac{q^2}{Mc^2}\right)^2 \frac{1}{\beta^2} \ln\left(\frac{Q_{\max}}{Q_{\min}}\right)$$

Comment on frequency dependence --

Original expression for radiation intensity:

$$\frac{d^2I}{d\omega d\Omega} = \frac{q^2}{4\pi^2 c} \left| \int dt e^{i\omega(t - \hat{r} \cdot \mathbf{R}_q(t)/c)} \frac{d}{dt} \left[\frac{\hat{r} \times (\hat{r} \times \boldsymbol{\beta})}{1 - \hat{r} \cdot \boldsymbol{\beta}} \right] \right|^2$$

In the previous derivations, we have assumed that $\omega(t - \hat{r} \cdot \mathbf{R}_q(t)/c) \ll 1$.

$$\omega(t - \hat{r} \cdot \mathbf{R}_q(t)/c) = \omega \left(t - \hat{r} \cdot \int_0^t dt' \boldsymbol{\beta}(t') \right) \approx \omega \tau (1 - \hat{r} \cdot \langle \boldsymbol{\beta} \rangle)$$

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Differential radiation cross section - - continued

Radiation cross section in terms of momentum transfer

$$\frac{d\chi}{d\omega} = \int_{Q_{\min}}^{Q_{\max}} dQ \frac{d^2\chi}{d\omega dQ} = \frac{16}{3} \frac{(Ze)^2}{c} \left(\frac{q^2}{Mc^2} \right)^2 \frac{1}{\beta^2} \ln \left(\frac{Q_{\max}}{Q_{\min}} \right)$$

Note that: $Q^2 = 2p^2(1 - \cos\theta') \Rightarrow Q_{\max} = 2p$

In general, Q_{\min} is determined by the collision time

$$\text{condition } \omega\tau < 1 \Rightarrow Q_{\min} \approx \frac{2Ze q \omega}{v^2}$$

Radiation cross section for classical non - relativistic process

$$\frac{d\chi}{d\omega} = \frac{16}{3} \frac{(Ze)^2}{c} \left(\frac{q^2}{Mc^2} \right)^2 \frac{1}{\beta^2} \ln \left(\frac{\lambda M v^3}{Ze q \omega} \right) \quad \lambda = \text{"fudge factor" of order unity}$$

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