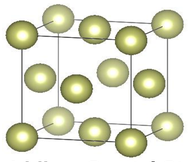
Surface Structure Determination of Iridium (111) using μLEED-*IV* Dynamical Analysis

Ben MacDonald | Advisors: Karsten Pohl, University of New Hampshire | Zhongwei Dai, now Brookhaven National Lab

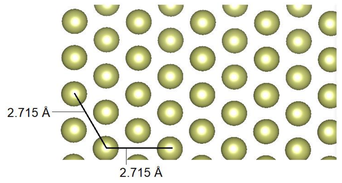
University of New Hampshire

Introduction

Iridium (Ir) is a transition metal, atomic number 77, with face center cubic (fcc) crystal structure. The lattice constant of the (111) surface of Iridium is close to that of graphene, making it a strong candidate for studying the growth mechanism of graphene.

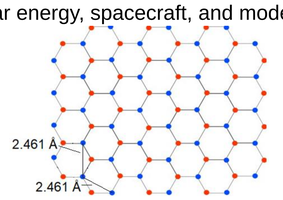


Bulk Iridium Crystal Structure



Iridium (111) Face Top View

Graphene is a two dimensional material made of a single layer of carbon atoms in a honeycomb structure. Graphene has potential revolutionary applications in solar energy, spacecraft, and modern electronics.



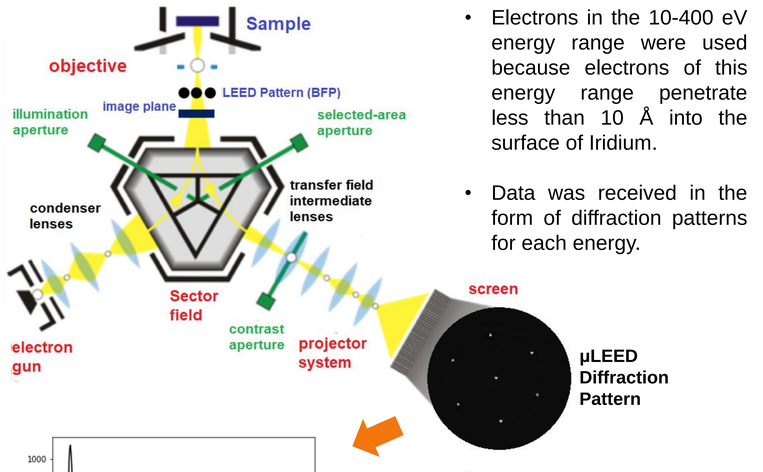
Graphene Crystal Structure

Iridium has a lattice constant of 2.715 Å [1], and graphene 2.461 Å [2], so it is expected that the graphene structure on Ir (111) will differ slightly from its isolated form.

To understand the growth of graphene on Iridium, we need to understand the surface structure of Iridium (111), specifically how the interlayer spacing differs from the bulk value of 2.217 Å [1]. This was accomplished here using micro Low Energy Electron Diffraction Intensity vs Energy (μLEED-*IV*) Dynamical Analysis.

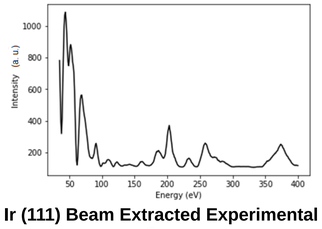
Experiments and Data Acquisition

Low Energy Electron Microscopy System

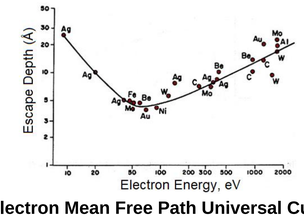


- Electrons in the 10-400 eV energy range were used because electrons of this energy range penetrate less than 10 Å into the surface of Iridium.
- Data was received in the form of diffraction patterns for each energy.

μLEED Diffraction Pattern



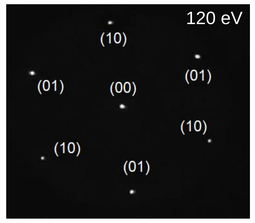
Ir (111) Beam Extracted Experimental *IV* Curve



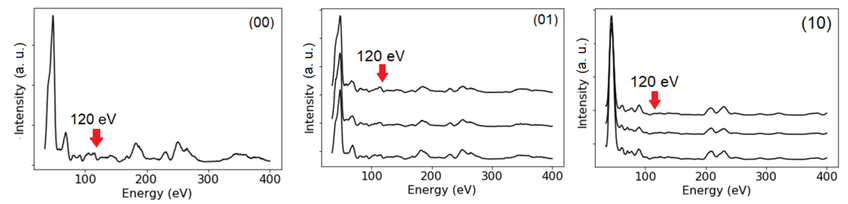
Electron Mean Free Path Universal Curve

Results and Analysis

LEED Experimental Diffraction Pattern and Extracted *IV* Curves



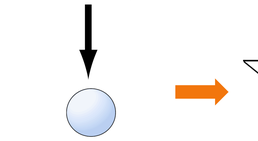
LEED Diffraction Pattern at 120 eV



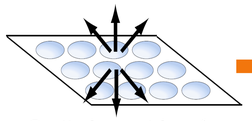
Extracted *IV* Curves; note the lower relative intensity of the (10) curves at 120 eV, corresponding to the dimmer diffraction points at that energy

- *IV* curves were extracted via the intensity of pixels at diffraction points for each energy
- There were diffraction images for each energy ranging from about 10 eV to 400 eV, incrementing by 2 eV
- The Ir (111) three fold symmetry is shown in the three (01) and three (10) curves

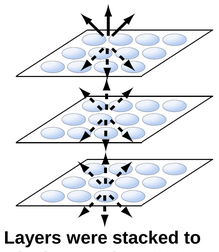
μLEED-*IV* Dynamical Analysis



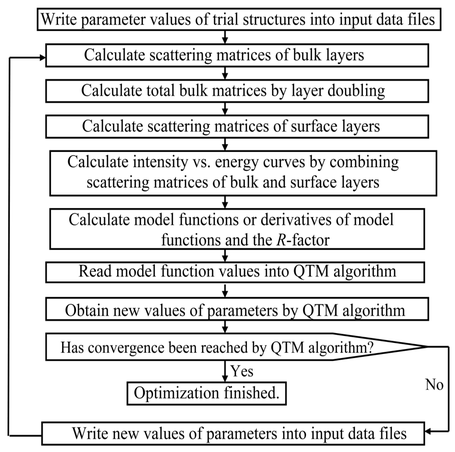
First, scattering of the electron by a single atom was calculated



Scattering matrices for each layer of atoms were calculated using the muffin tin model



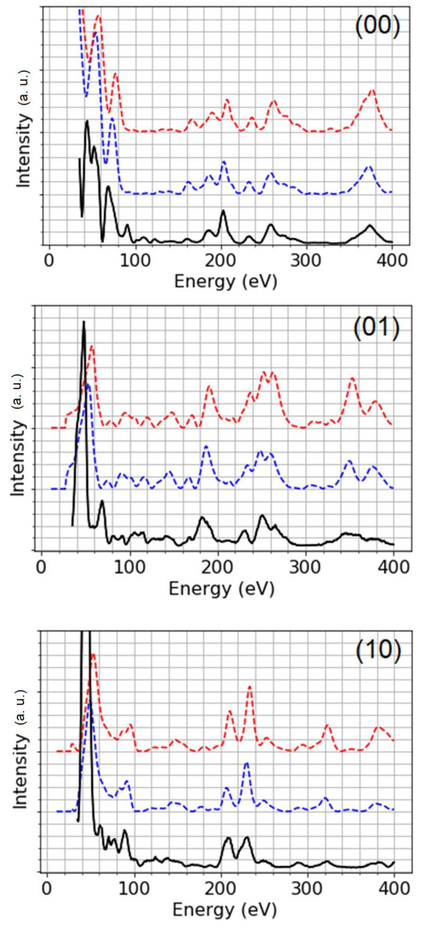
Layers were stacked to calculate total scattering matrix of the surface, from which the calculated *IV* curves were created



Optimization Algorithm Flowchart

- Calculations were done with programs described by Van Hove et al. [3] and Adams [4].
- Programs are written in FORTRAN and MS Visual Basic.
- Theoretical calculated *IV* curves were created based off characteristics of bulk Iridium. Some important input parameters used for Ir (111) were [1]:
  - Bulk interlayer spacing: d = 2.217 Å
  - 2-D lattice constants: $a = b$ = 2.715 Å
  - 3-fold symmetry (improves accuracy)
  - Atomic vibration: $\langle u^2 \rangle_T$ = 0.062 Å
  - Muffin tin constant = 5 eV
  - Atom coordinates

Experimental (black), Bulk Calculated (red), and Optimized (blue) *IV* curves.

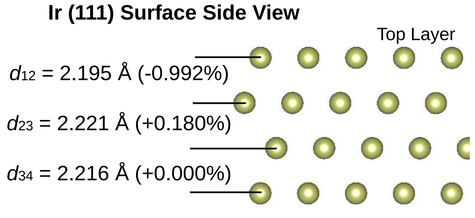


- The calculated curves were compared to the experimental curves and optimized using the Quadradic Tensor Method
- Agreement between calculated and experimental curves is represented by an R-factor
- An R-factor less than 0.1 represents a good agreement and a reliable structure determination.
- The optimized curves have an R-factor of 0.096. Comparatively, the R-factor for the un-optimized curves was 0.205.

Conclusions

Variable	Description	Initial Value	Optimized Value	Matsumoto
d_{12}	Distance between first and second layer	2.217 Å	2.195 Å	2.197 ± 0.014 Å
d_{23}	Distance between second and third layer	2.217 Å	2.221 Å	2.205 ± 0.019 Å
d_{34}	Distance between third and fourth layer	2.217 Å	2.216 Å	2.233 ± 0.023 Å

Ir (111) Surface Side View



- Optimized interlayer spacings all agree well with the findings in Matsumoto et Al. [5], giving further confidence in this calculation, along with our R-factor of 0.096.
- Success in the surface structure determination of Ir (111) encourages further investigation of the graphene grown on Ir (111) structure. This work is on-going.

References

[1] C.M. Chan, S.L. Cunningham, M.A. Van Hove, W.H. Weinberg, S.P. Withrow. (1977). An analysis of the structure of the iridium (111) surface by low-energy electron diffraction. Surf. Sci., 66, p. 394
[2] Reddy, D., et. Al. (2011). Graphene field-effect transistors. Journal of Physics D: Applied Physics, 44(31).
[3] M. A. Van Hove, S. Y. Tong, (1979). Surface Crystallography by LEED, Springer-Verlag (Berlin),
[4] Adams, D. L. (2002). A simple and effective procedure for the refinement of surface structure in LEED. Surface Science, 519(3),
[5] Matsumoto, M., et. Al. (2012). Dynamical LEED analyses of the clean and the NO-adsorbed Ir(111) surface. Surface Science, 606(19-20), 1489-1500.

Acknowledgements

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