

XPS analysis of pyrite thin films

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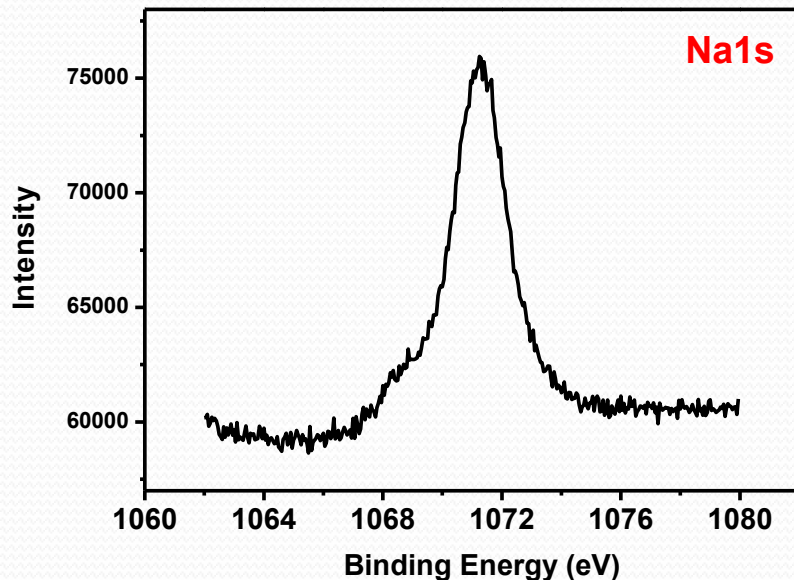
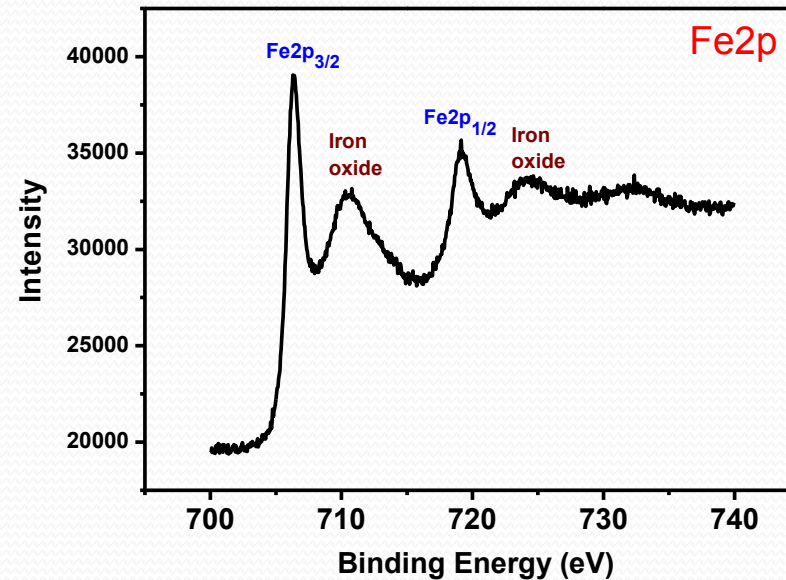
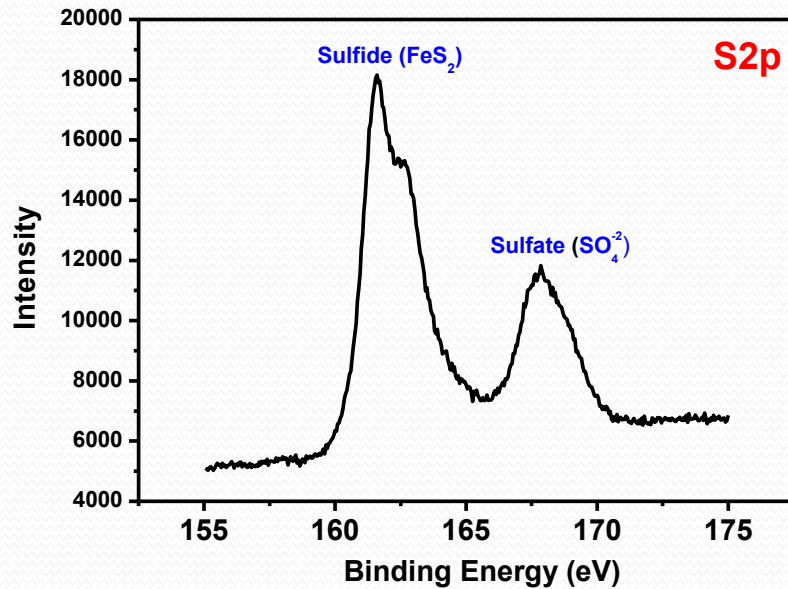
John C. Hemminger group

March 15, 2011

Outline

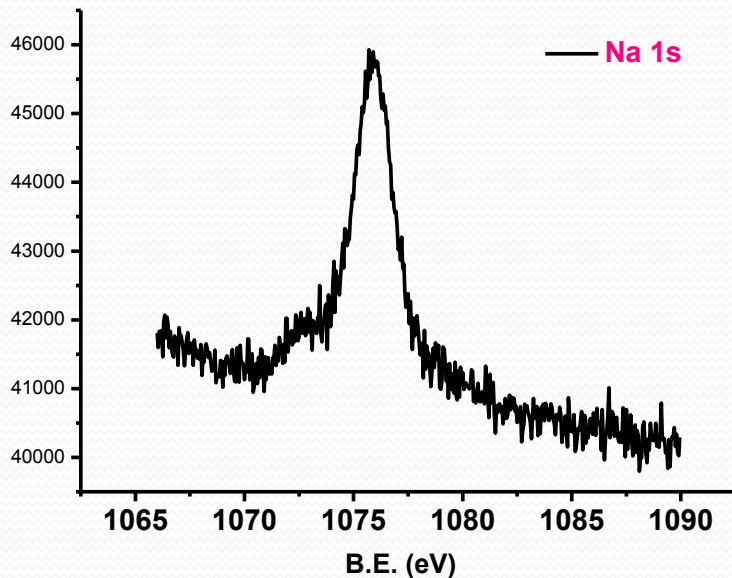
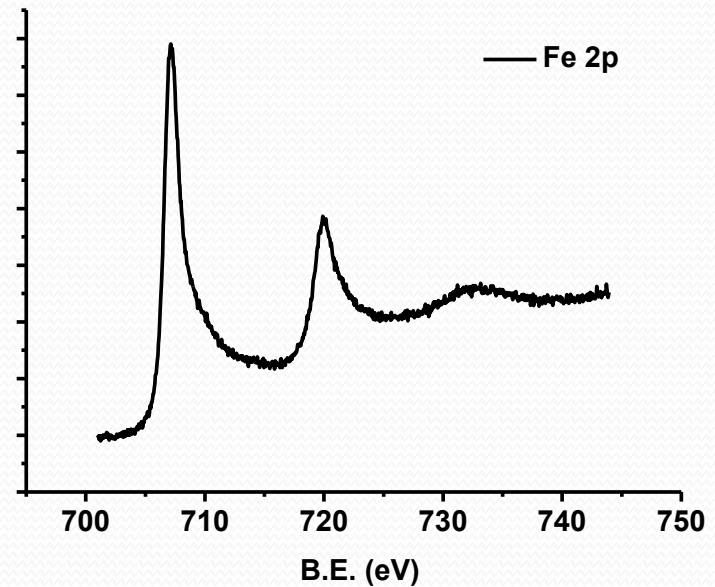
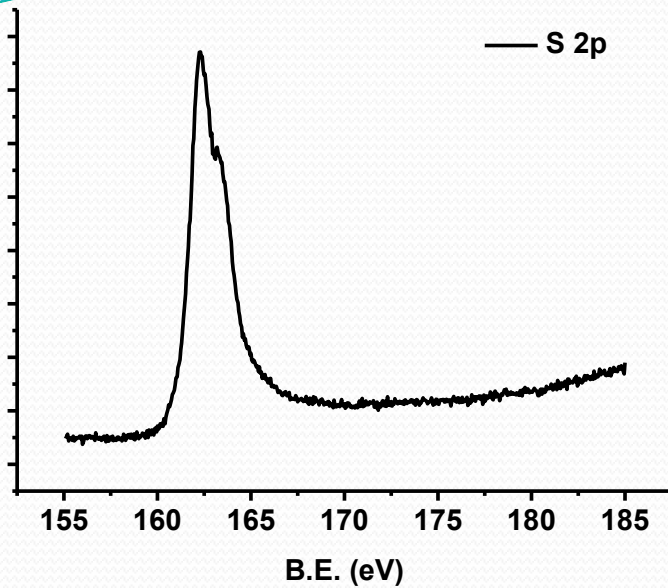
- Pyrite thin films on the **glass, ITO, Mo-glass, AF-32 (Alkali-free glass)**
 - How **Na** plays the role in growing pyrite thin film on the glass.
- Band gap determination for Pyrite thin films on Si
 - Valence band spectrum
 - Valence band spectrum + X-ray absorption spectrum (XAS)

Pyrite thin films on the glass **without** annealing in elemental sulfur condition



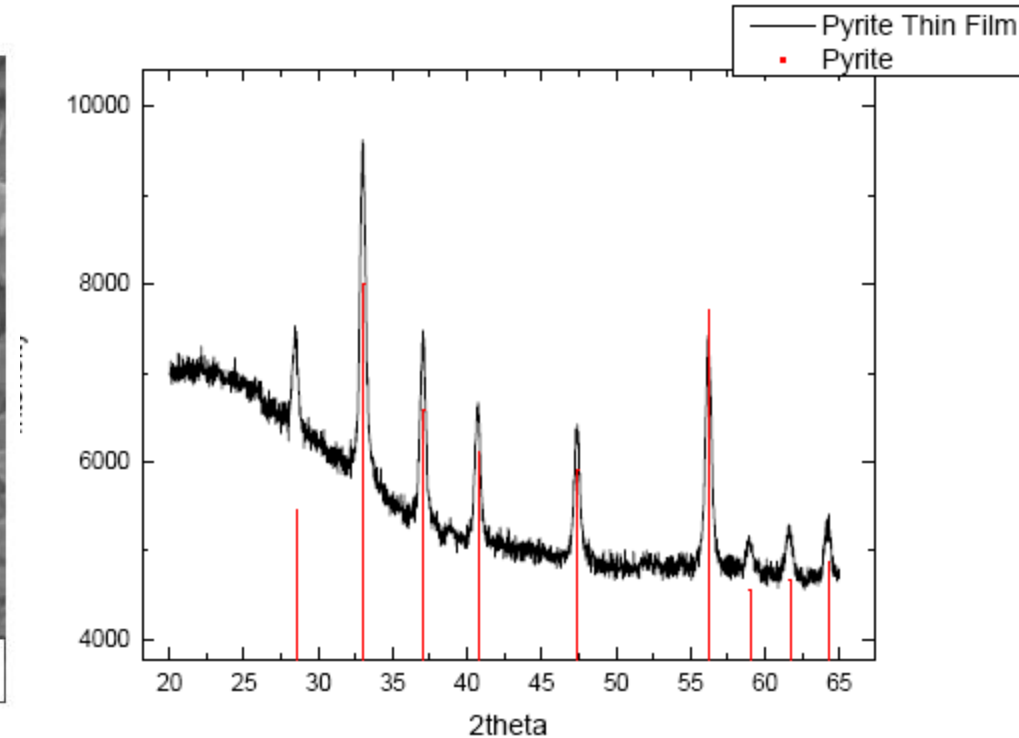
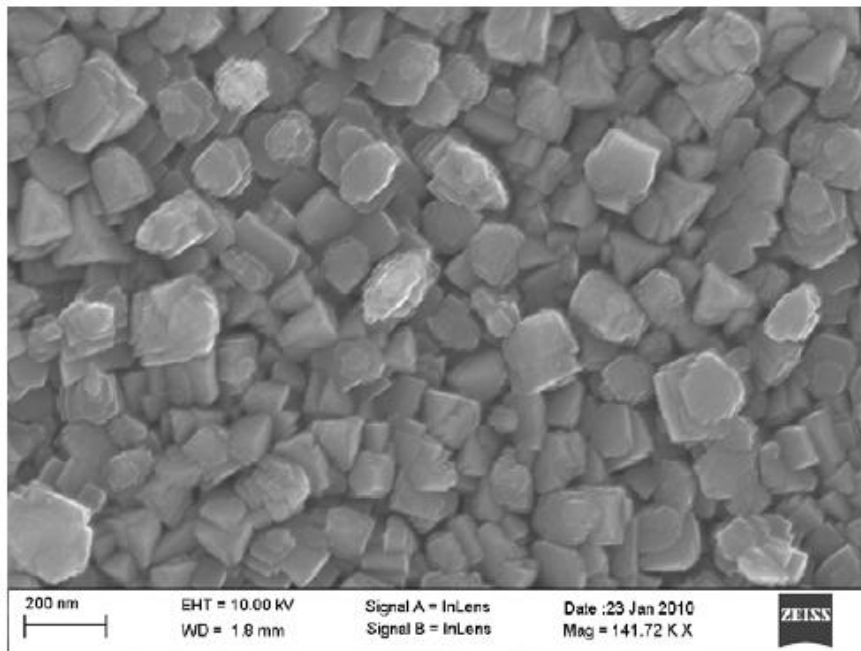
- The pyrite has been **oxidized**.
- **Na exists** on the surface of the pyrite thin film.

Fresh Pyrite thin films on the glass



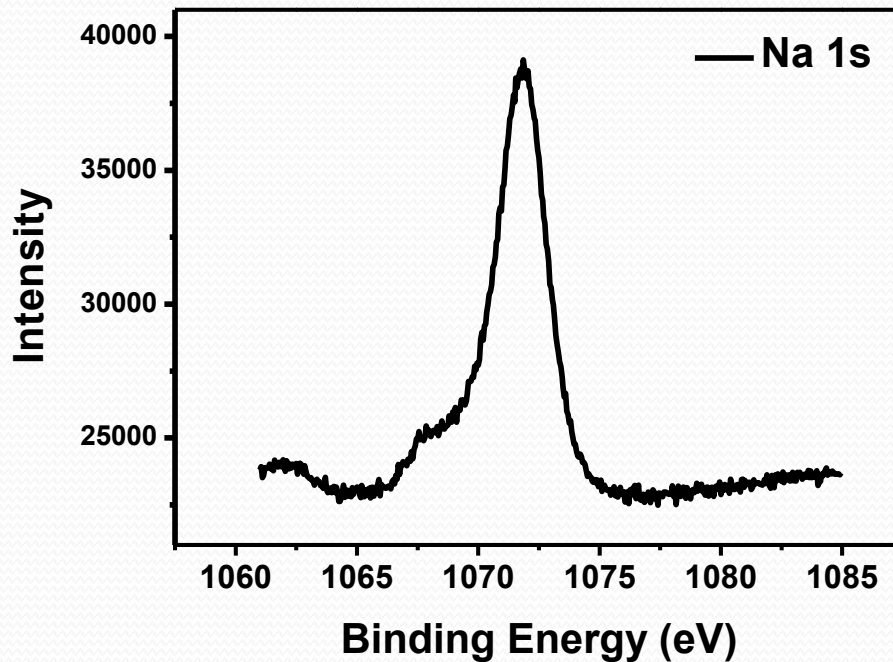
- No oxidation occurs on the surface of fresh pyrite.
- **Na** really exists on the surface.

SEM and XRD of pyrite on the glass



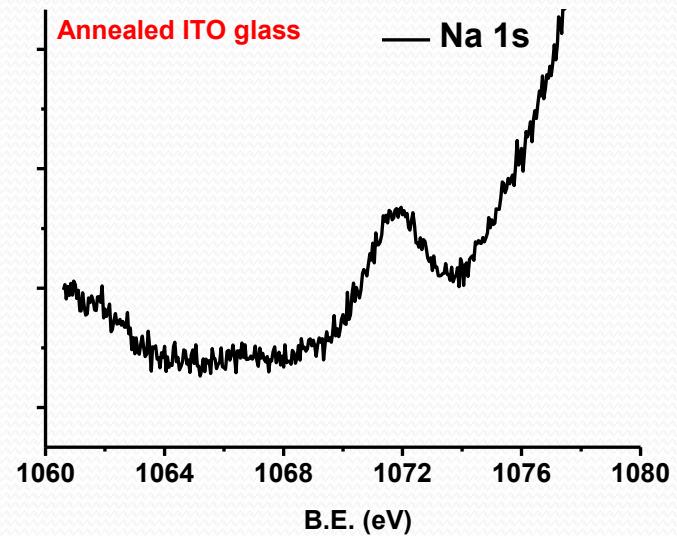
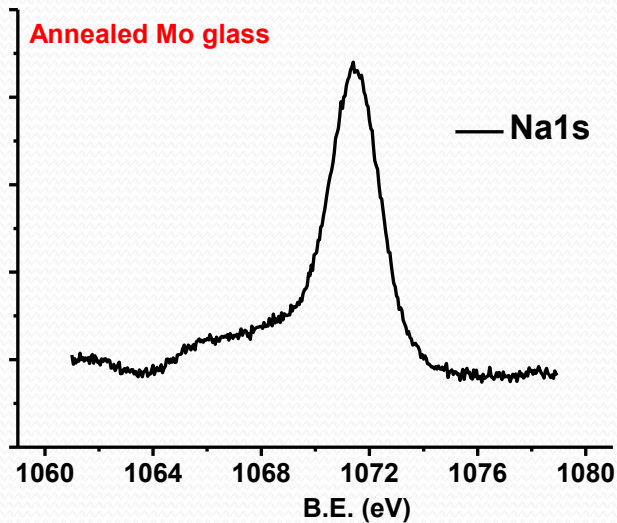
Na 1s spectrum for the blank annealed glass

Where did Na come from ??

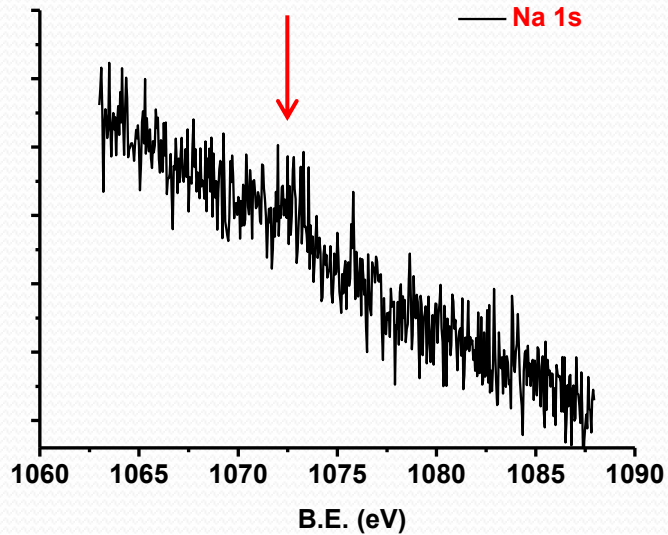
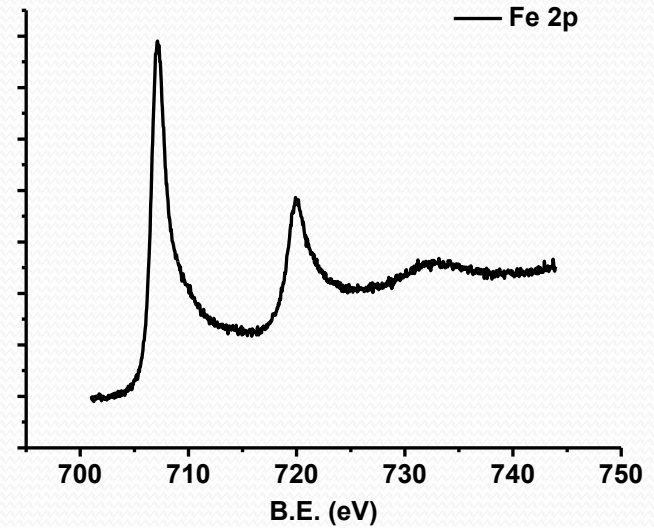
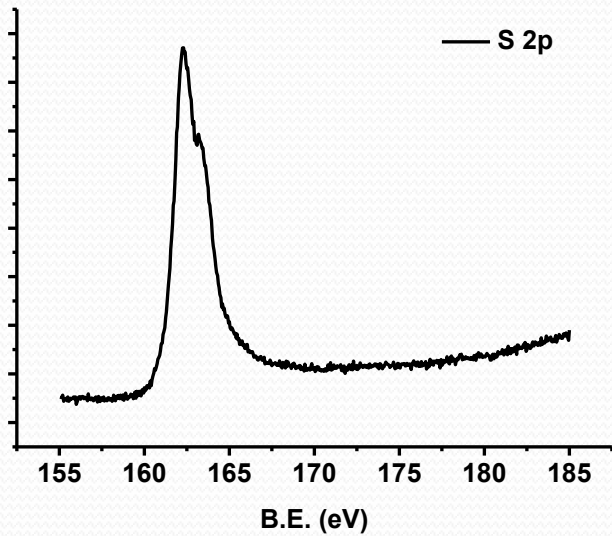


Na comes from the glass substrate and leaches into the pyrite thin films.

Na 1s Mo-glass V.S Annealed ITO

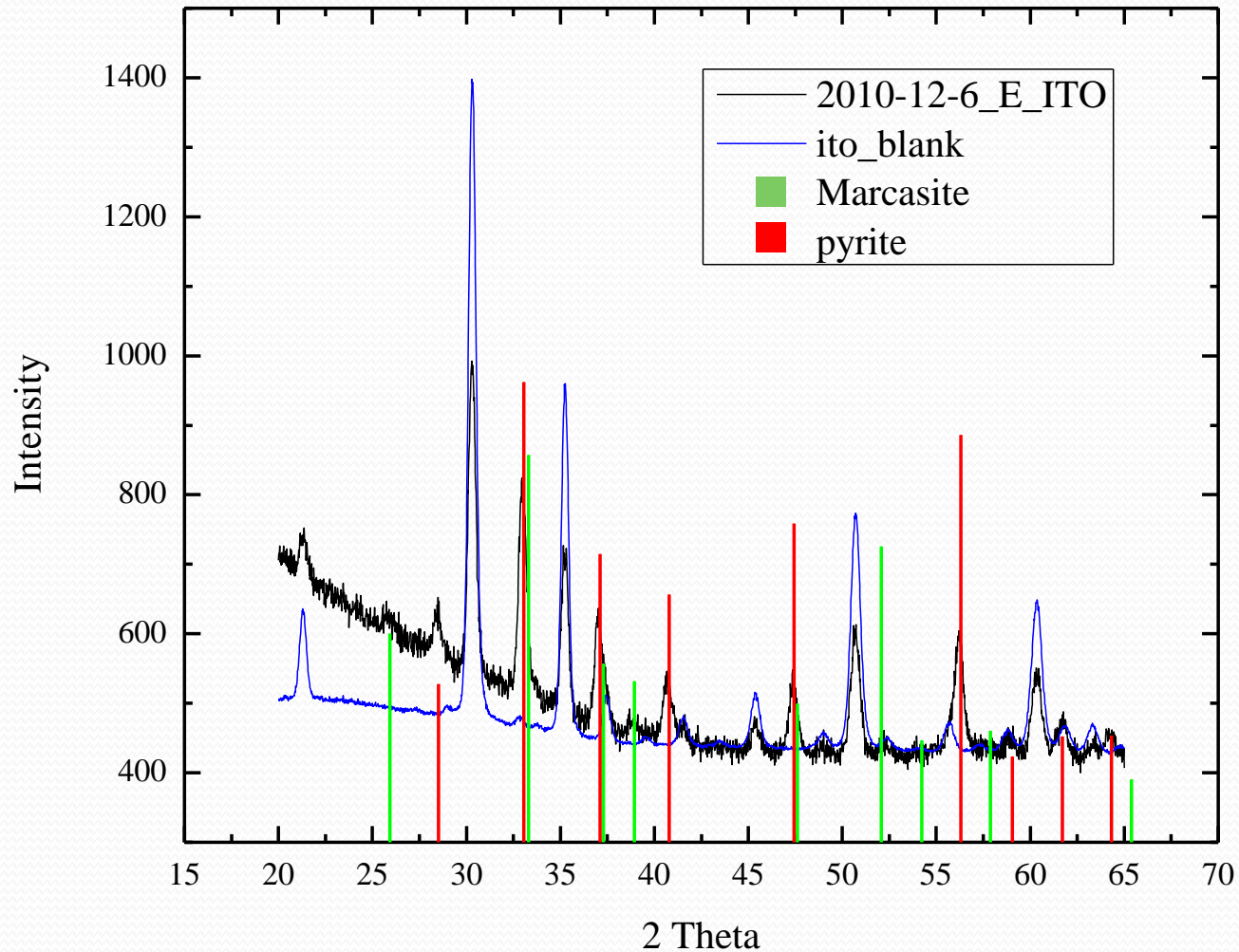


Fresh Pyrite thin films on the ITO glass

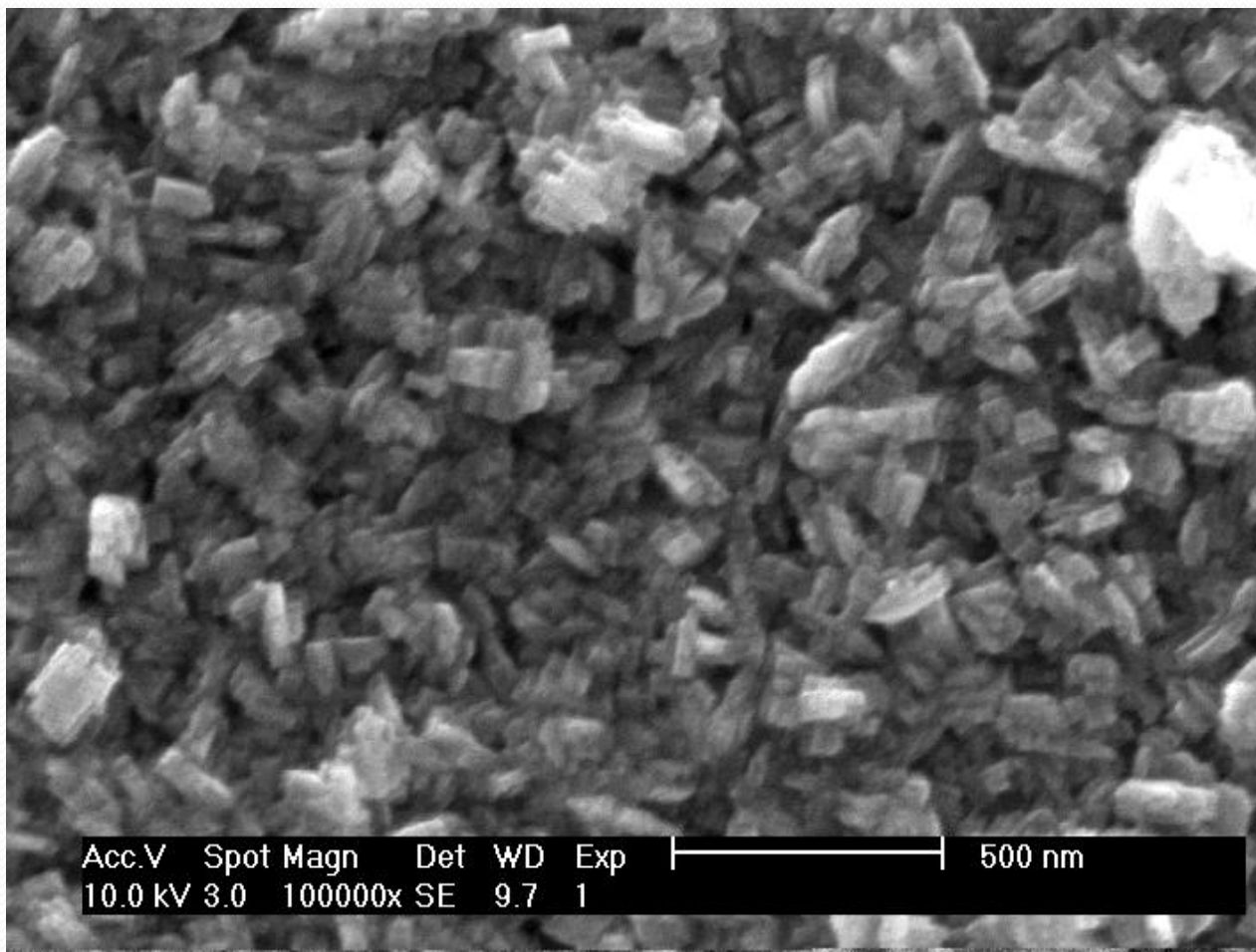


It appears to be a little amount of **Na** still on the surface.

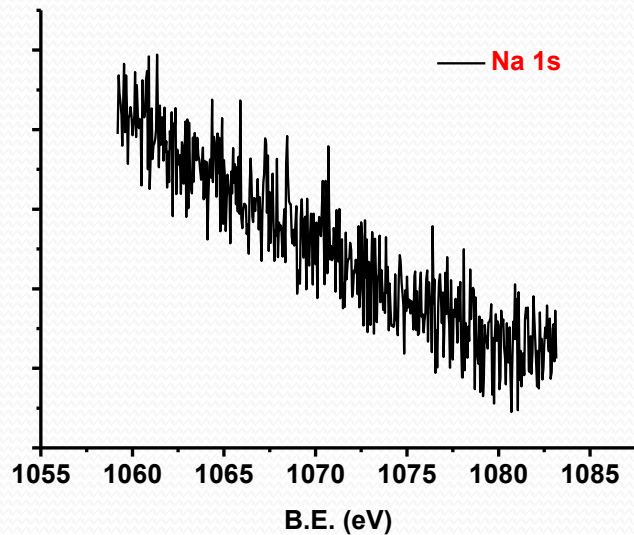
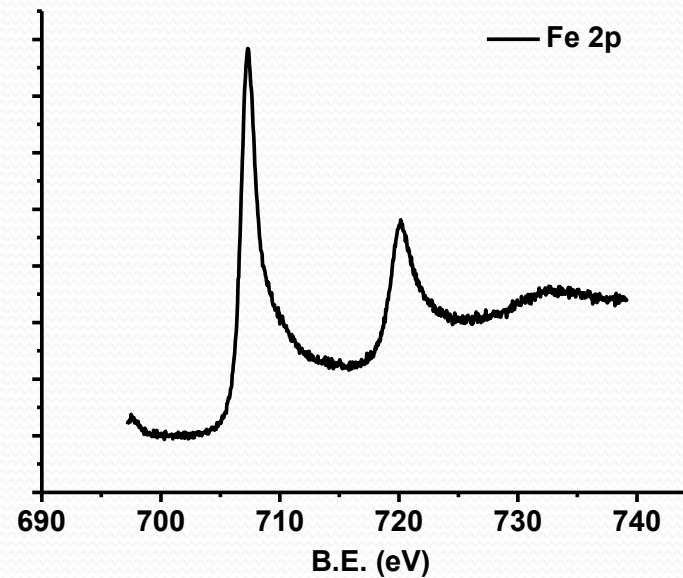
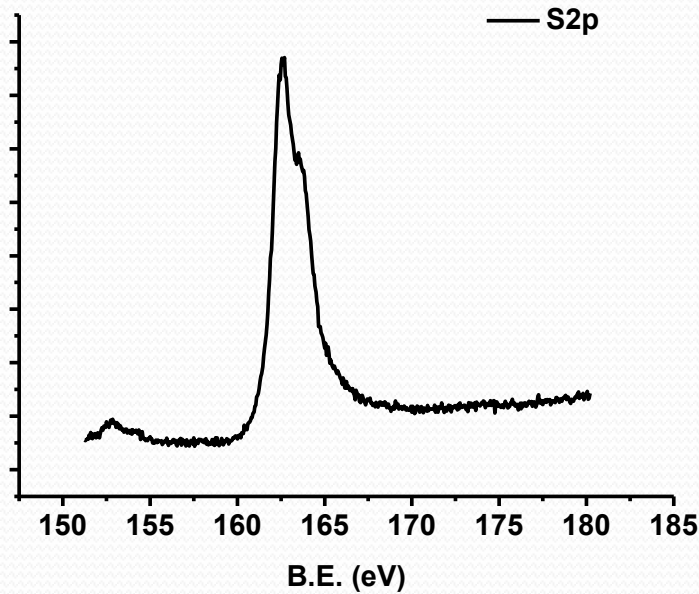
AcAc/TBDS Growth on ITO



AcAc/TBDS Growth on ITO

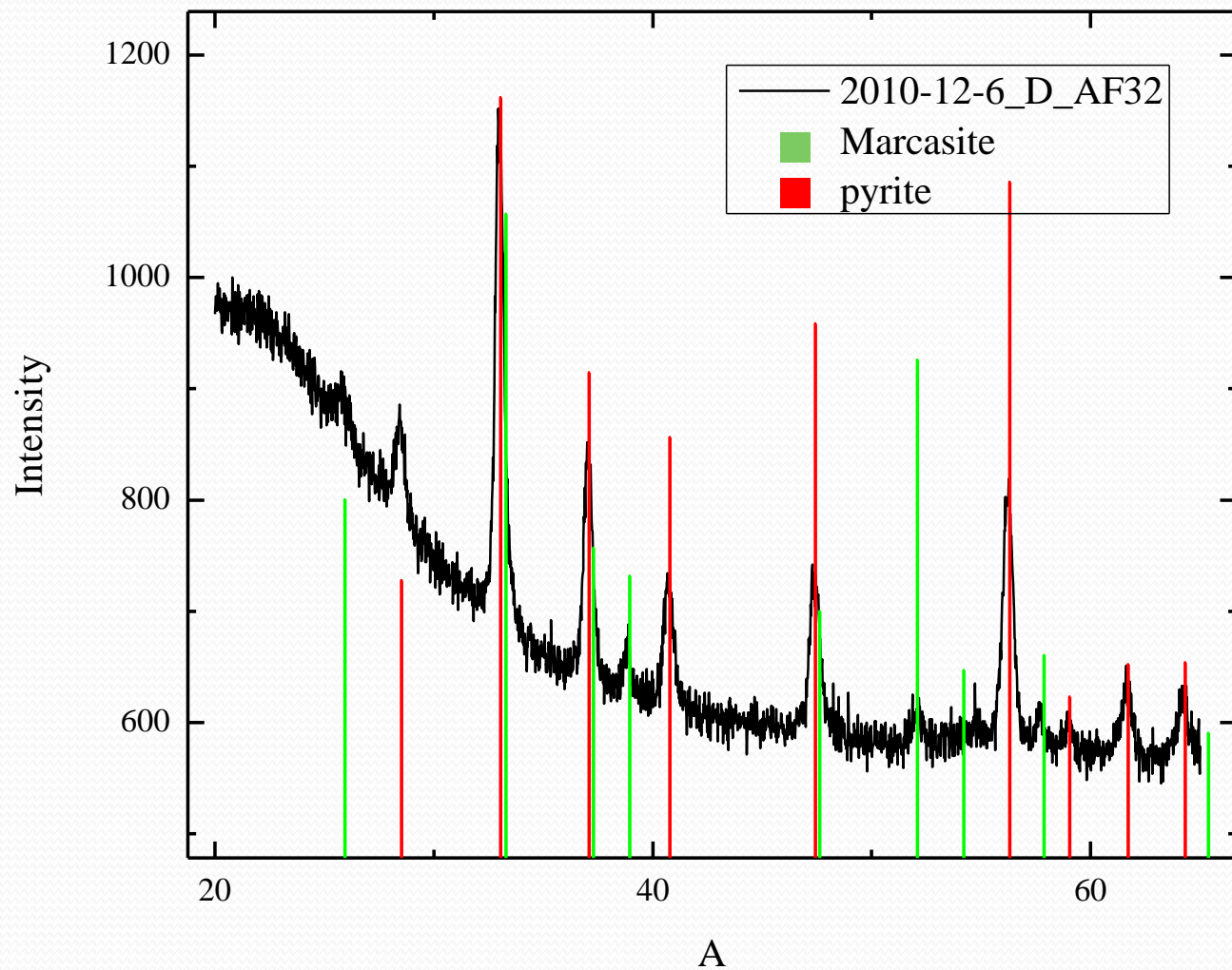


Fresh Pyrite thin films on the AF-32 glass (alkali free glass)

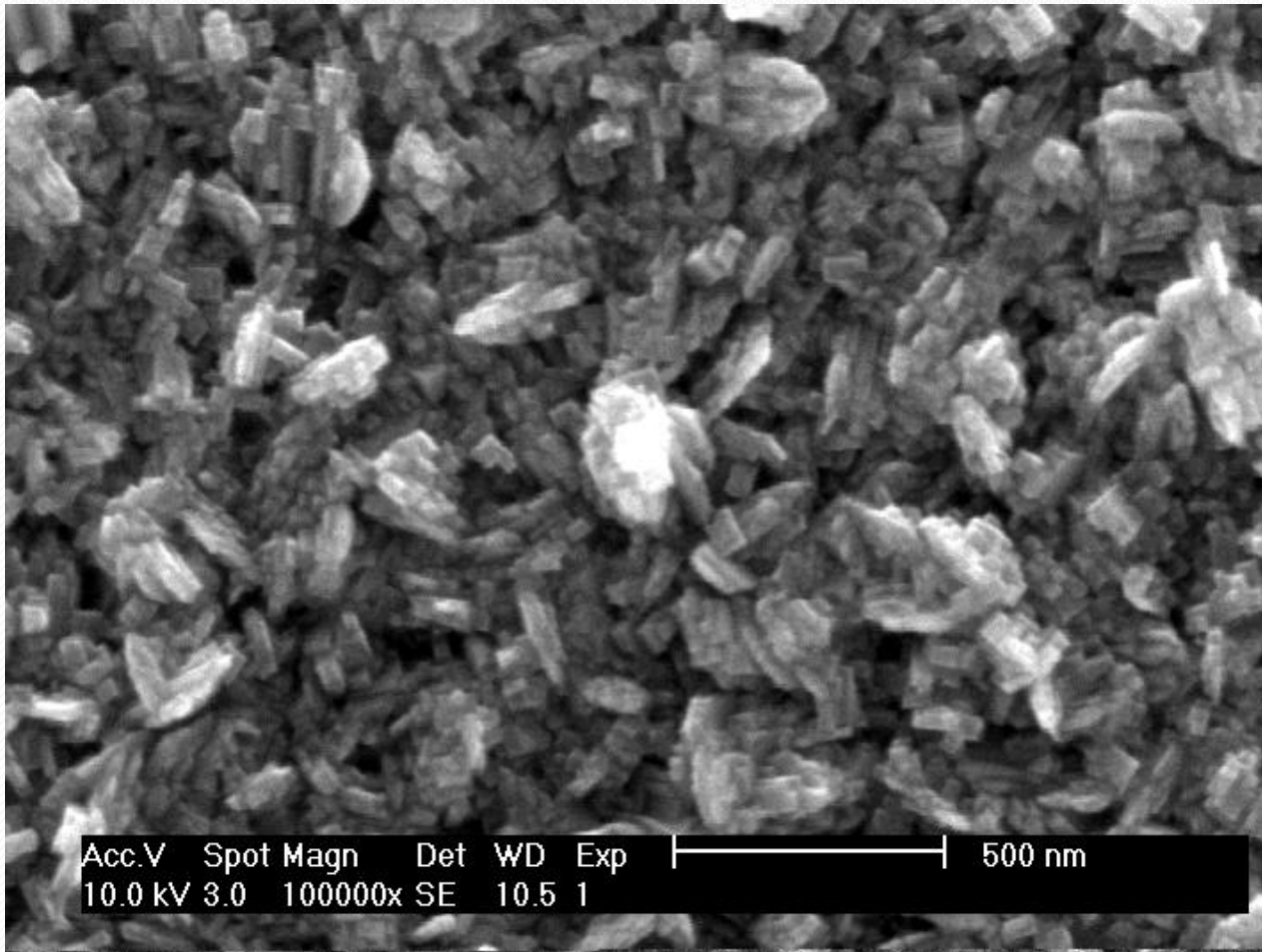


It appears to be **no** Na leaches into the pyrite thin film.

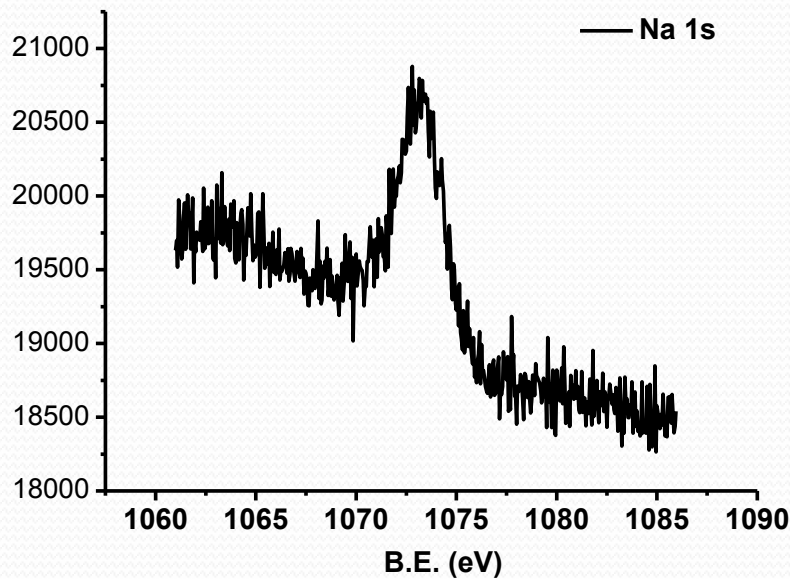
AcAc/TBDS Growth on AF32



AcAc/TBDS Growth on AF32

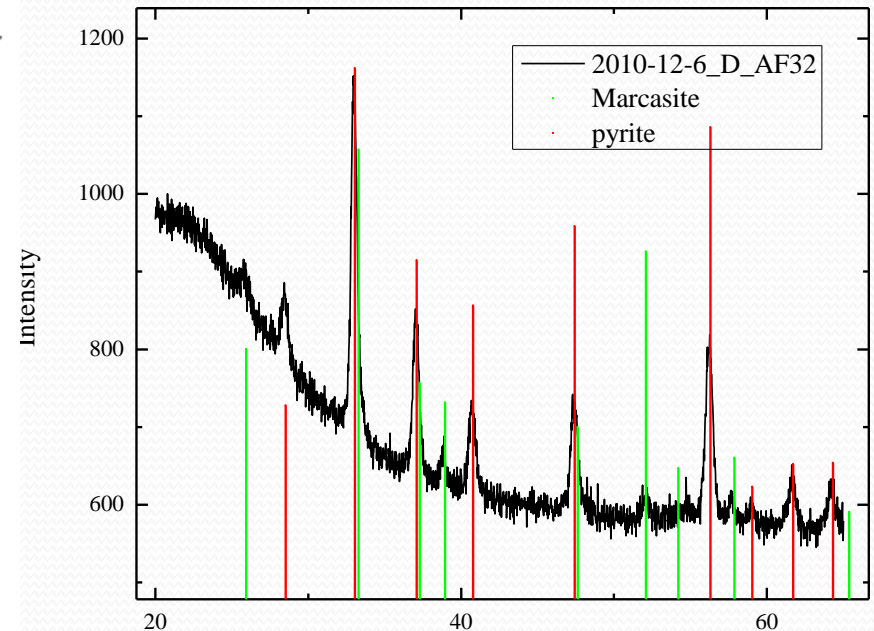
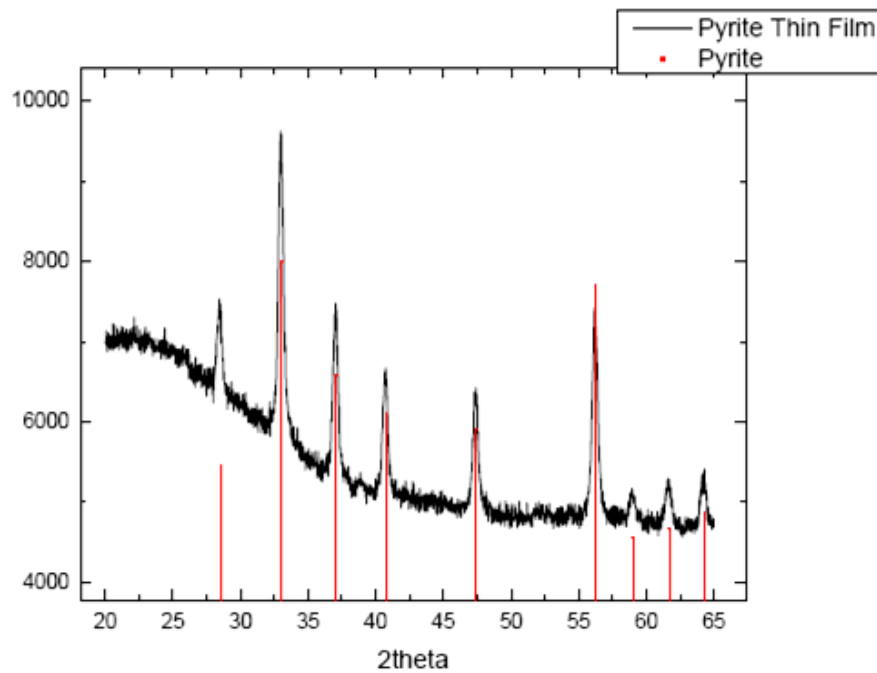
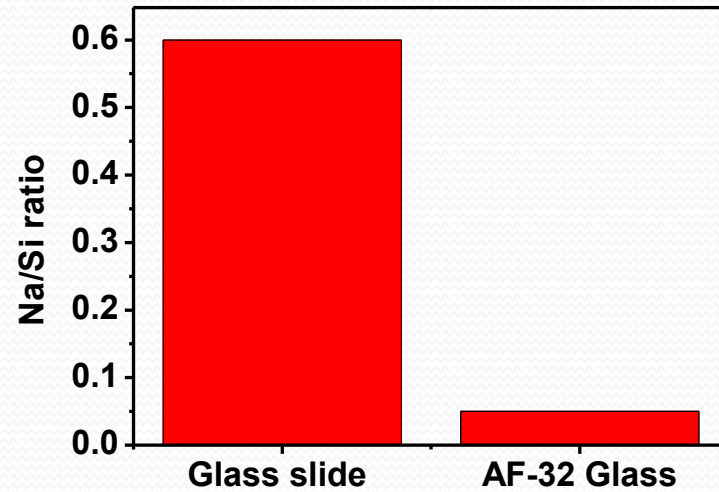


Na 1s spectrum for the blank annealed AF-32 glass



Alkali-free is **NOT** really alkali-free
From commercial AF-32 glasses.

Na concentration V.S. degree of crystalline pyrite



Take-home messages

- **The source of Na** in pyrite thin films comes from glass substrates.
- AF-32 glass is **NOT** a alkali-free glass.
- The glass substrate with **well-controlled Na concentration** is needed to further clarify how Na plays the role in growing of pyrite thin films on the glass.