On the possibility of positive ion detection in gaseous TPCs

LIOR ARAZI

WEIZMANN INSTITUTE OF SCIENCE

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Motivation: accurate track reconstruction in rare-event searches

How accurate?

$$\sigma_{ions} = \sqrt{2Dt} = \sqrt{\frac{2k_BT}{q_e} \cdot \frac{L}{E}} = 0.225\sqrt{\frac{L}{E}} \quad \left(\sigma \,\&\, L \; in \; cm, E \; in \frac{V}{cm}\right)$$

E.g. 10 bar Xe, E = 300 V/cm

$$\sigma_{ions} = \begin{cases} 1.3\;mm & L = 1\;m \\ 1.8\;mm & L = 2\;m \end{cases}$$

Electron diffusion under the same conditions:

$$\sigma_{electrons} \approx \begin{cases} 13\;mm & L = 1\;m \\ 18\;mm & L = 2\;m \end{cases}$$

Problem: ions are slow

Drift velocity of $\mathcal{O}(10^2)$ cm/s, thermal kinetic energies

⇓

Detection must rely on a **potential-driven** process

Luckily, Nature provided us with Auger neutralization (AN)

What is AN?

- When a positive ion approaches a surface a first electron tunnels out and neutralizes it, leaving the system with excess energy
- This energy is simultaneously transferred, in an Auger-like process, to a second electron which may be emitted into the gas

Historical context

- First suggested by S. S. Shekhter in 1937
- Experimental and theoretical foundations laid by H. D. Hagstrum (Bell Labs) in 1953-1961: studied AN for single ions of all noble gases, impinging on metals (W, Mo) and semiconductors (Si, Ge)
- Was of central importance to the development of plasma panel displays
- Still an active field in surface science theory

Key features of AN

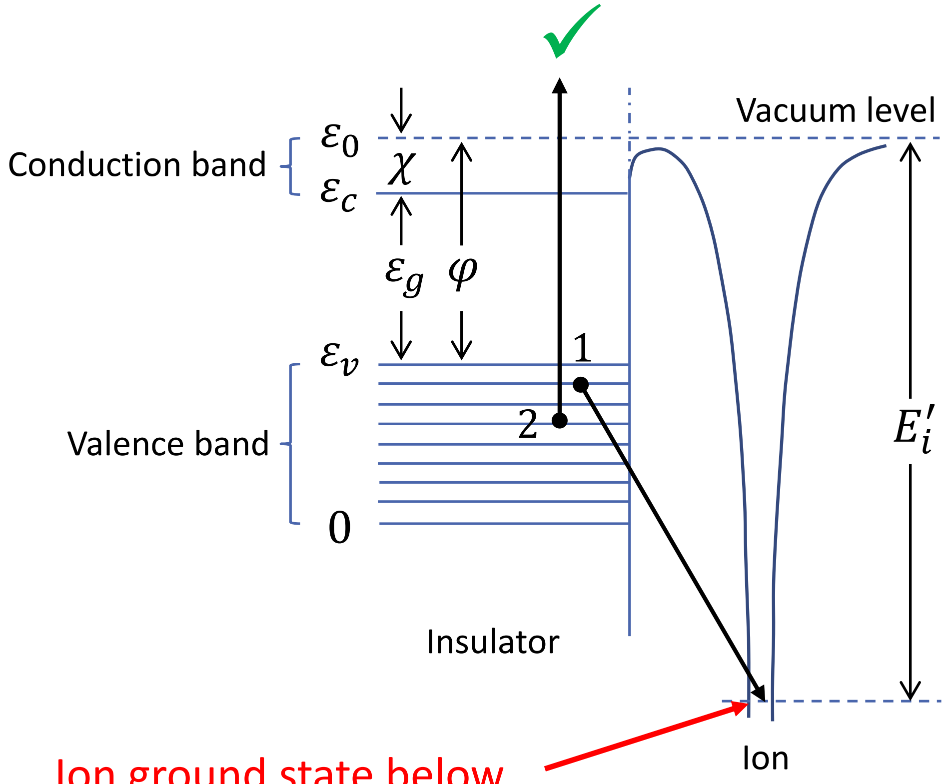
- Driven by potential energy → ok for thermal ions
- Occurs for both atomic and molecular ions
- Occurs for metals and insulators/semiconductors
- Necessary condition: the ionization energy of the ion close to the surface must be larger than twice the work function: $E_i' > 2\varphi$
- γ_i : secondary electron yield = probability of ion-induced secondary electron emission (IISEE)
- γ_i generally increases with increasing E_i' and decreasing φ. Can be as large as tens of %

Other mechanisms?

- In some cases AN is the *only* possible mechanism for charge transfer (e.g., He^+ on metals and semiconductors). This requires that the ion ground and excited states are not resonant with occupied states in the solid.

- When resonant processes are possible secondary electron emission can still occur, but with lower probabilities. The condition $E_i' > 2\varphi$ still holds.

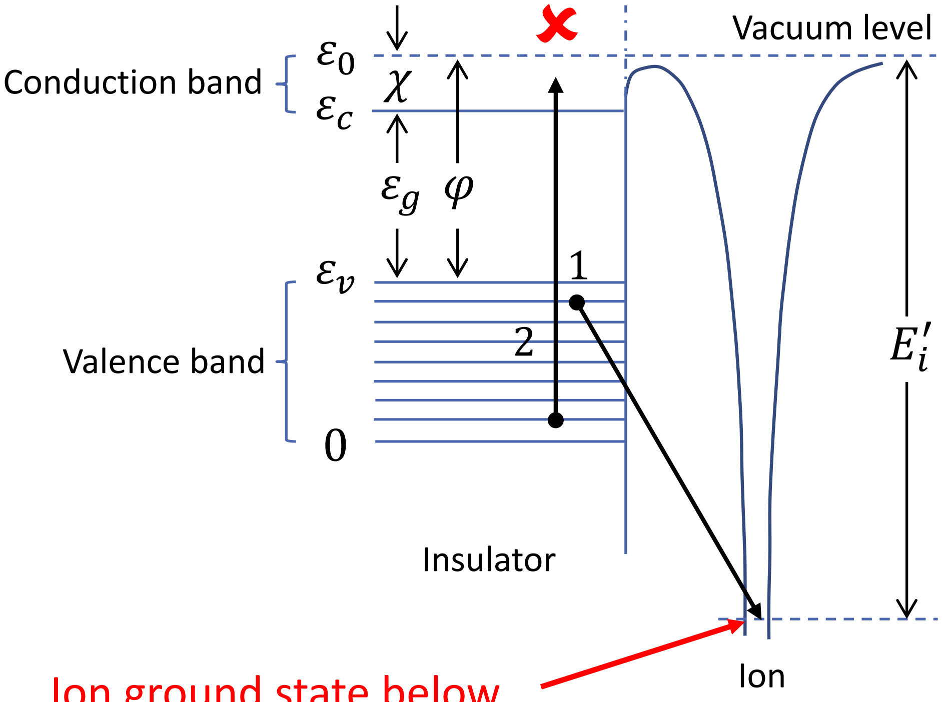
Auger neutralization – external emission



Ion ground state below bottom of valence band

- Energy lost by electron 1 is taken by electron 2
- If sufficiently large and electron 2 starts from the upper valence band it may be emitted externally

Auger neutralization – internal emission



Ion ground state below bottom of valence band

- If electron 2 starts from the lower valence band it may enter the conduction band without external emission
- Also useful?

S. Shchemelinin and A. Breskin, “Observation of electron excitation into silicon conduction band by slow-ion surface neutralization”, arXiv:1607.02924

IISEE yields of noble gas ions

Target: atomically clean molybdenum, work function 4.3 eV

ion	$E_i [eV]$	$E_i - 2\varphi [eV]$	$\gamma_i [\%]$
He^+	24.59	16.0	30
Ne^+	21.56	13.0	25.4
Ar^+	15.76	7.2	12.2
Kr^+	14.00	5.4	6.9
Xe^+	12.13	3.5	2.2

Monolayer of N_2 on W reduces γ_i by a factor ranging from 1.6 (He) to 6.5 (Xe)

H. D. Hagstrum, Phys Rev 104 (1956) 672

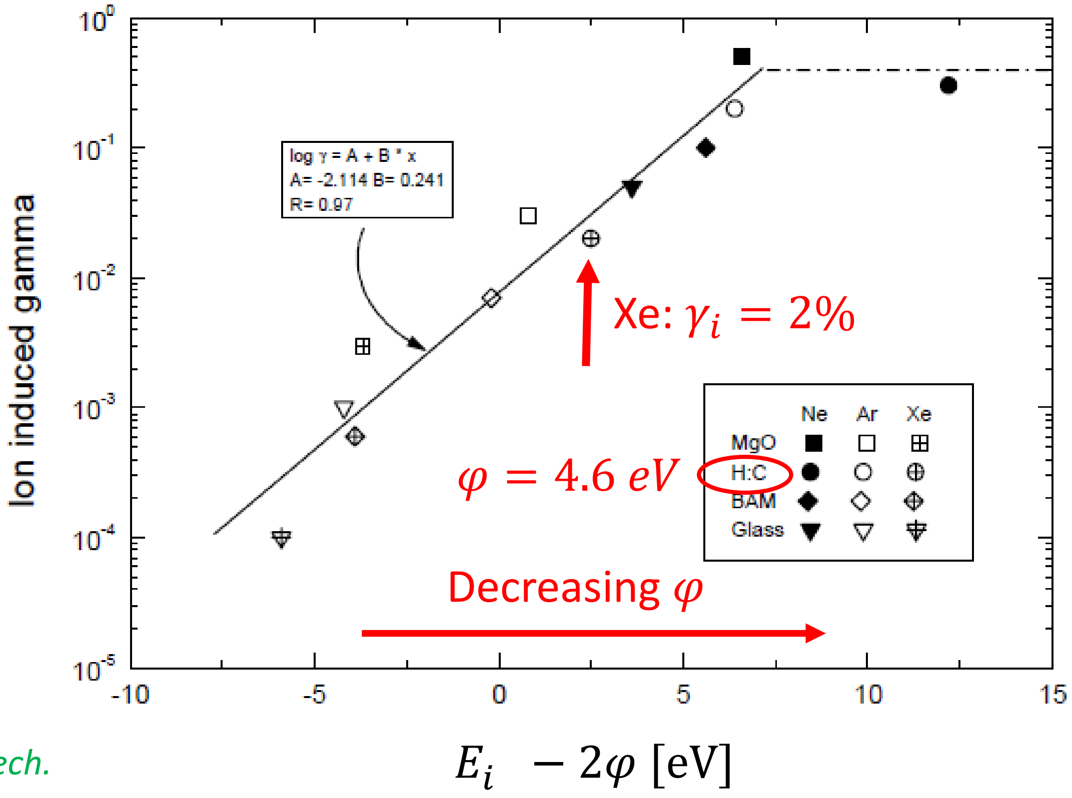
IISEE yields of noble gas ions

γ_i inferred from Paschen curves

H:C = Hydrogen terminated CVD diamond, with Negative Electron Affinity (NEA) of -0.8 eV

BAM = $BaMgAl_{10}O_{17}$ phosphor

Further decrease of φ in NEA-diamond expected to result in larger γ_i for Xe



Xe: $\gamma_i = 2\%$

$\varphi = 4.6\ eV$

Decreasing φ

$E_i - 2\varphi$ [eV]

Elsbergen et al, *SID Int. Symp. Dig. Tech. Papers*, 2000, 220–223.

So – how about xenon?

Searching for $\beta\beta0\nu$ in HPXe at the ton scale → compromise between energy resolution and accuracy in track reconstruction

Design option	Intrinsic FWHM Energy resolution	rms diffusion (1 m)	rms diffusion (2 m)
Pure Xe	0.33%	$\sim 13\ mm$	$\sim 18\ mm$
Xe + 0.05% CO_2	0.47%	$4.8\ mm$	$6.8\ mm$
Xe + 0.5% CH_4	0.53%	$3.1\ mm$	$4.4\ mm$
Xe + 1.0% CH_4	0.8%	$2.3\ mm$	$3.2\ mm$
Pure Xe using ions for topology and electrons for energy	0.33%	$1.3\ mm$	$1.8\ mm$

*

* Azevedo et al, JINST 11 (2016) C02007 arXiv:1511.07189 – 10 bar, 300 V/cm

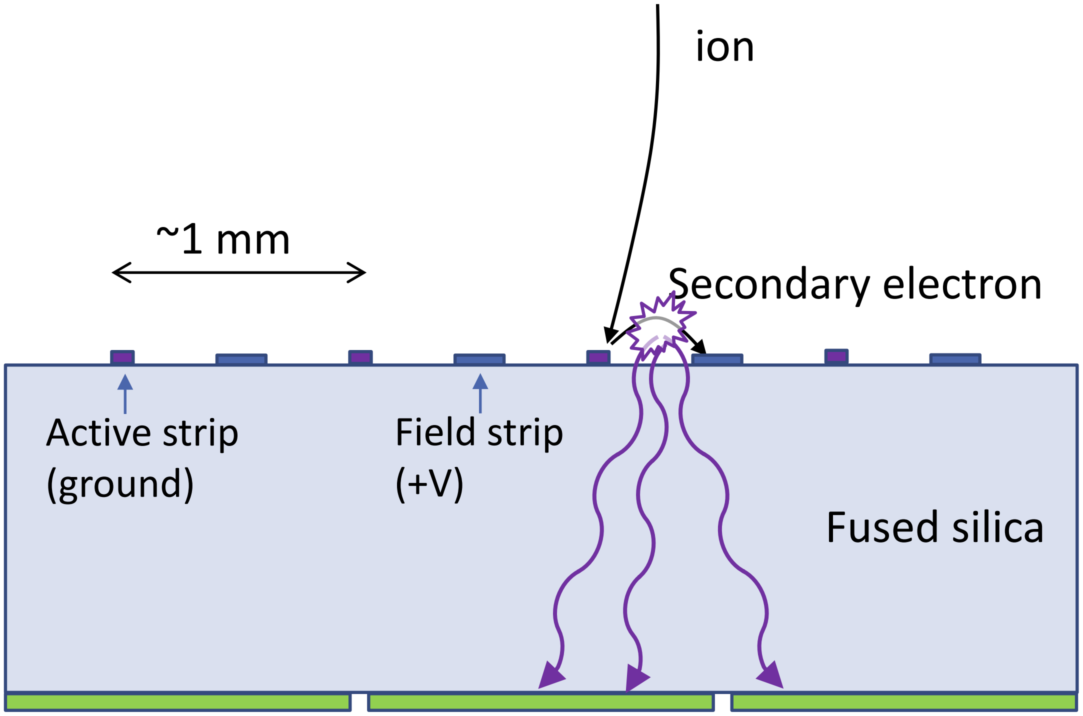
Let's take this one step at a time

- $1 \cdot 10^5$ electron-ion pairs for event at $Q_{\beta\beta}$
- All Xe^+ ions immediately ($\sim 10^{-10}$ s) convert to Xe_2^+
- Electrons quickly reach EL region near anode (at +HV)
- Energy + (smeared) track image measured by electrons EL signal
- Xe_2^+ ions reach cathode plane within <1 s
- Xe_2^+ ions ionization energy = 11.2 eV (lowest of all impurities) → no charge-exchange collisions → all Xe_2^+ ions make it to cathode

Now here comes the fun part

- Cathode plane comprised of tiled array of fused silica plates, each with MSGC-like pattern of active strips at ground, interlaced with field strips at modest +HV. Spacing between active strips ~1 mm.
- Ions landing on active strips release secondary electrons by AN
- Emitted electrons follow field lines to positive field strips. Field tuned to gain of $\mathcal{O}(10)$ → $\mathcal{O}(10^3)$ photons per detected ion
- EL light produced by electrons recorded by dense array of VUV-SiPMs immediately behind cathode plane
- Recorded light pattern provides track topology with spatial resolution governed by ion diffusion (+ some smearing by readout granularity)

Cathode plane cartoon



ion

~1 mm

Secondary electron

Active strip
(ground)

Field strip
(+V)

Fused silica

VUV sensitive SiPMs

Some numbers

- EL signals sufficiently large ($\mathcal{O}(10^3)$ photons)

$$\Downarrow$$

Ion Detection efficiency $= \gamma_{eff} = \gamma_i \cdot \varepsilon_{ext}$

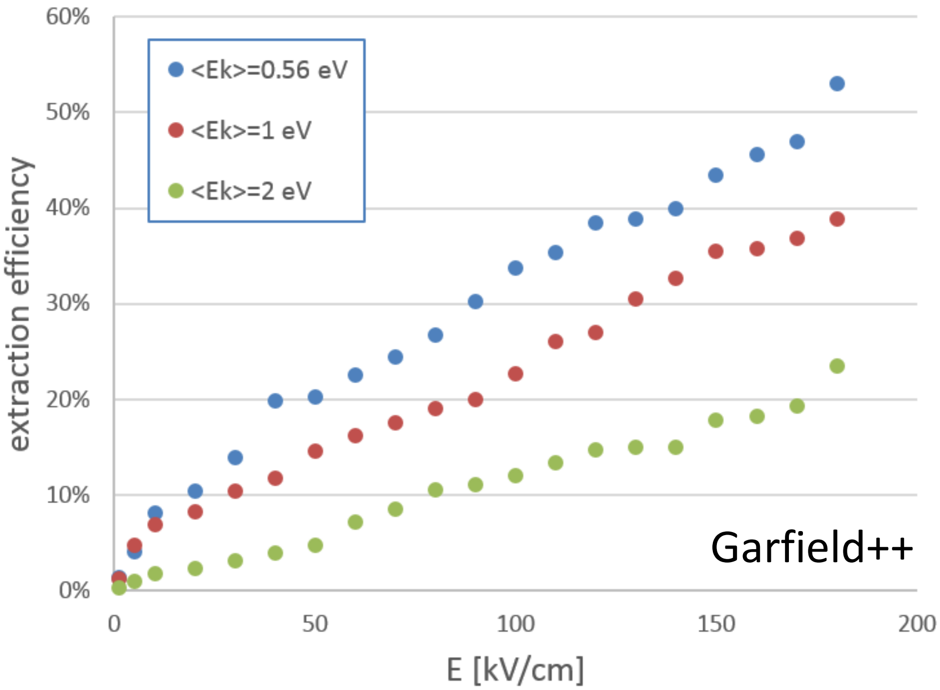
where ε_{ext} is the extraction efficiency = probability that the emitted electron is not backscattered to the surface

- ε_{ext} can be readily >20% → γ_i of a few % will provide several hundred detected ions (out of $1 \cdot 10^5$)
- E.g. $\gamma_i = 2\%$ & $\varepsilon_{ext} = 20\%$ → 400 detected ions with ~0.5 mm spacing for 20 cm track

Extraction efficiency of electrons into 10 bar Xe at room temperature

For $E_i' = 10 - 11$ eV,
$\varphi = 3 - 4$ eV :

$$\langle E_k \rangle \approx \frac{1}{3} E_k^{max} \approx 0.6 - 1.6 \text{ eV}$$



Some more numbers

- For 6 mm SiPMs with array PDE=10%, 3 mm behind the cathode plane, the emission of 2000 EL photons into 4π gives $\sigma_{xy} \approx 0.5\ mm$ for center-of gravity (COG) determination
- For avalanche gain = 10, the required EL is then ~200 photons/e over a trajectory of ~0.5-1 mm (NEXT-100 TDR: 2500 photons/e over 5 mm)
- To avoid continuous ion feedback we need $gain \cdot \gamma_{eff} < 1$ – readily satisfied for gain of $\mathcal{O}(10)$ and $\gamma_{eff} < 1\%$
- EL signals will last $\mathcal{O}(10 - 100\ ns)$. Contribution of SiPM dark counts (even if 10^5 Hz/mm^2) will be small over the total area of the SiPM pixels used for COG
- EL photon feedback expected to be low (for active material of low QE and thin strips)
- **BUT: Field emission must be kept very low (roughly <10^{-14} A/cm^2)**

Candidate materials

CVD diamond with negative electron affinity (NEA)

- Either nanoparticles (UNCD – ultrananocrystalline diamond) or single-crystal layers
- ‘Tunable’ NEA depends on surface termination (e.g. by H, D or Mg) and annealing → work function can be tuned to 3-4 eV

  (at $\varphi = 4.6\ eV$ $\gamma_i = 2\%$ for Xe ions; naively $\varphi = 3\ eV$ → $\gamma_i \approx 10\%$)
- Passivation through surface termination → no monolayer of impurities
- Can be used to form thin strips on fused silica
- Field emission may be high for UNCD (much less for single-crystal layers), but can possibly be kept low enough by tweaking the parameters

Candidate materials

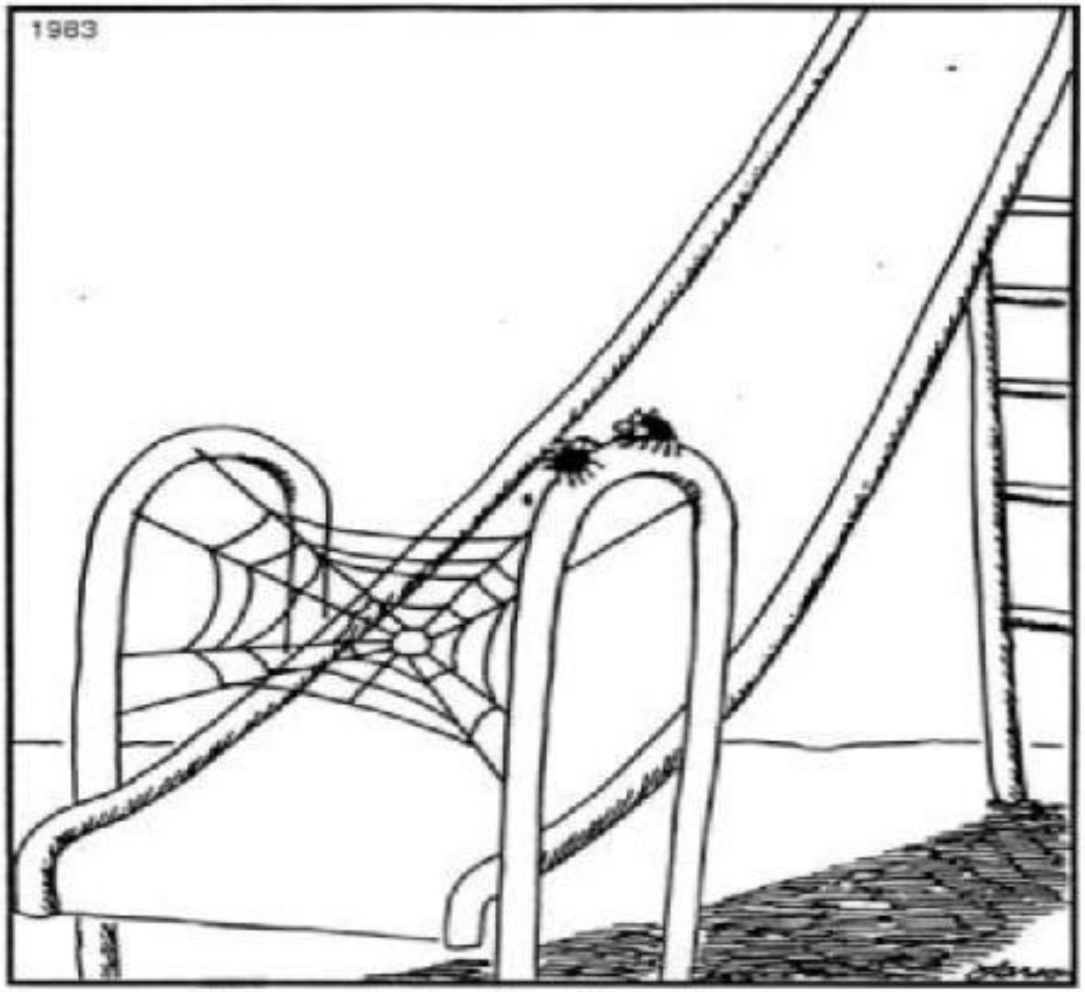
Thin MgO film on molybdenum

- Few atomic layers of MgO grown on single-crystal Mo
- Work function 3.2 eV
- Passivation provided by MgO → no monolayer of impurities
- No known issues with field emission

Stuckenholz et al, J. Phys. Chem. C 2015, 119, p. 12283

Summary and outlook

- Positive ion detection in ton-scale $\beta\beta0\nu$ searches in HPXe may enable having both superb intrinsic energy resolution (0.3% FWHM at $Q_{\beta\beta}$) and accurate track reconstruction ($\sigma < 1.8$ mm over 2 m drift)
- It will also enable having a t_0 signal from S1 (likely lost for Xe + admixtures)
- Since we start with 10^5 ions a modest IISEE yield of a few % will be sufficient for detecting several hundred ions with sub-mm spacing → should be enough to identify the two blobs + other track features
- Such yields appear at hand using existing materials (but must keep an eye on field emission)
- First samples for testing are expected soon from Argonne National Laboratory
- Careful studies required to translate this to actual sensitivity to $\beta\beta0\nu$
- Can AN be also used in directional dark matter searches?



“If we pull this off, we’ll eat like kings.”

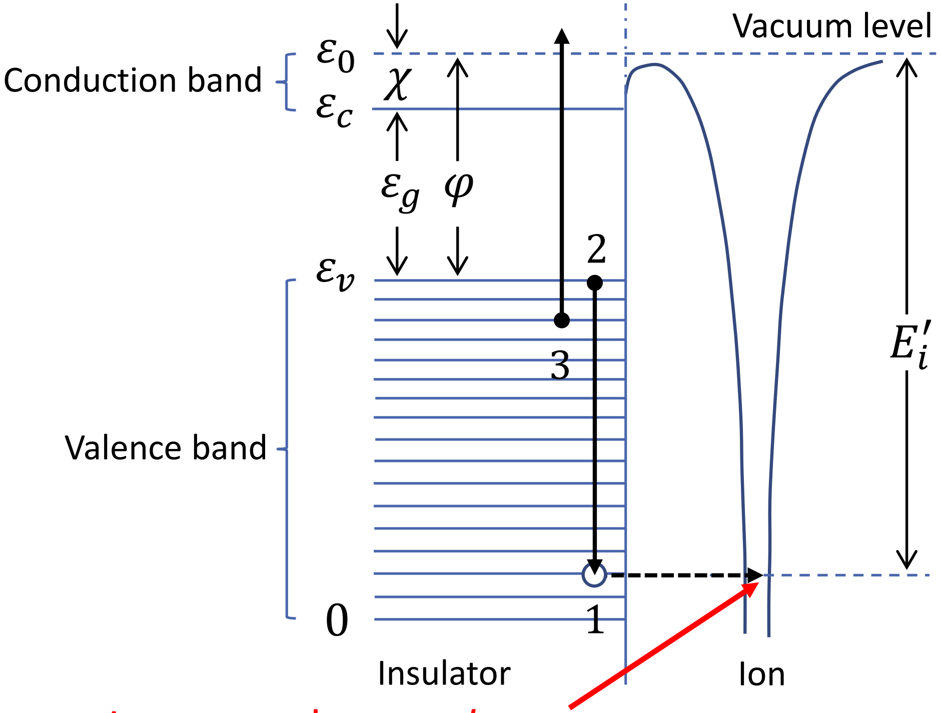
G. Larson, “The Far Side” (1983)

Backup slides

Resonance neutralization

- Dominant when the ground state of the ion lies above the bottom of the valence band (in insulators)
- A first valence electron tunnels resonantly to the ion ground state and neutralizes it, without losing energy
- A second valence electron drops to fill the hole left by electron 1
- The energy lost by electron 2 can be taken by a third electron only if it puts it in the conduction band (and may then be emitted) – otherwise it will be lost through other channels.
- Electron emission out of the solid still requires $E_i' > 2\varphi$ and happens with lower probability than the pure AN case.

Resonance neutralization – external emission



Ion ground state *above* bottom of valence band

If the energy lost by electron 2 as it drops to fill the hole is large enough, electron 3 can make it out.

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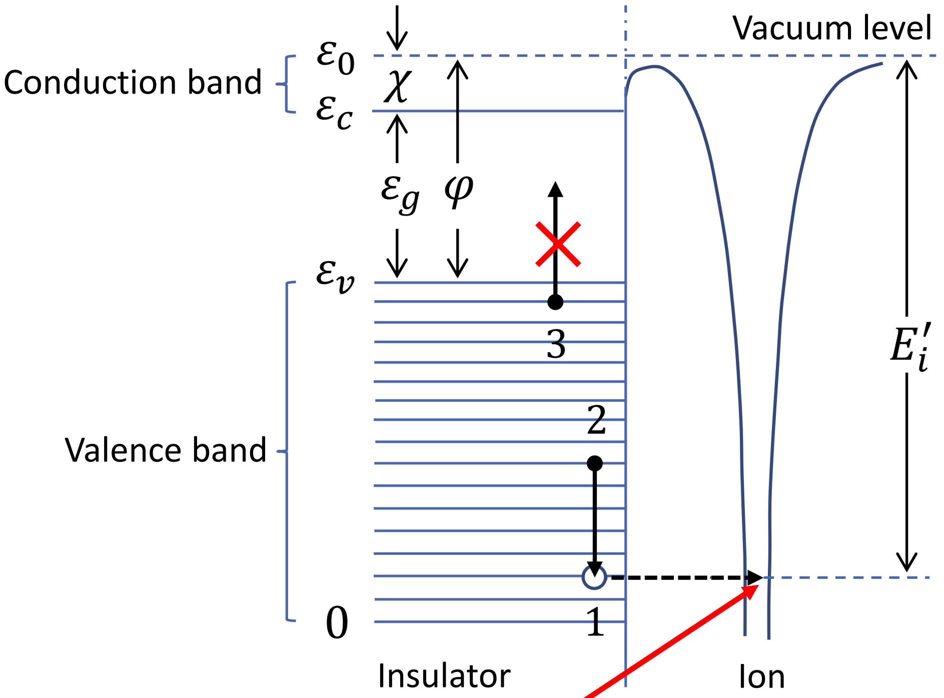
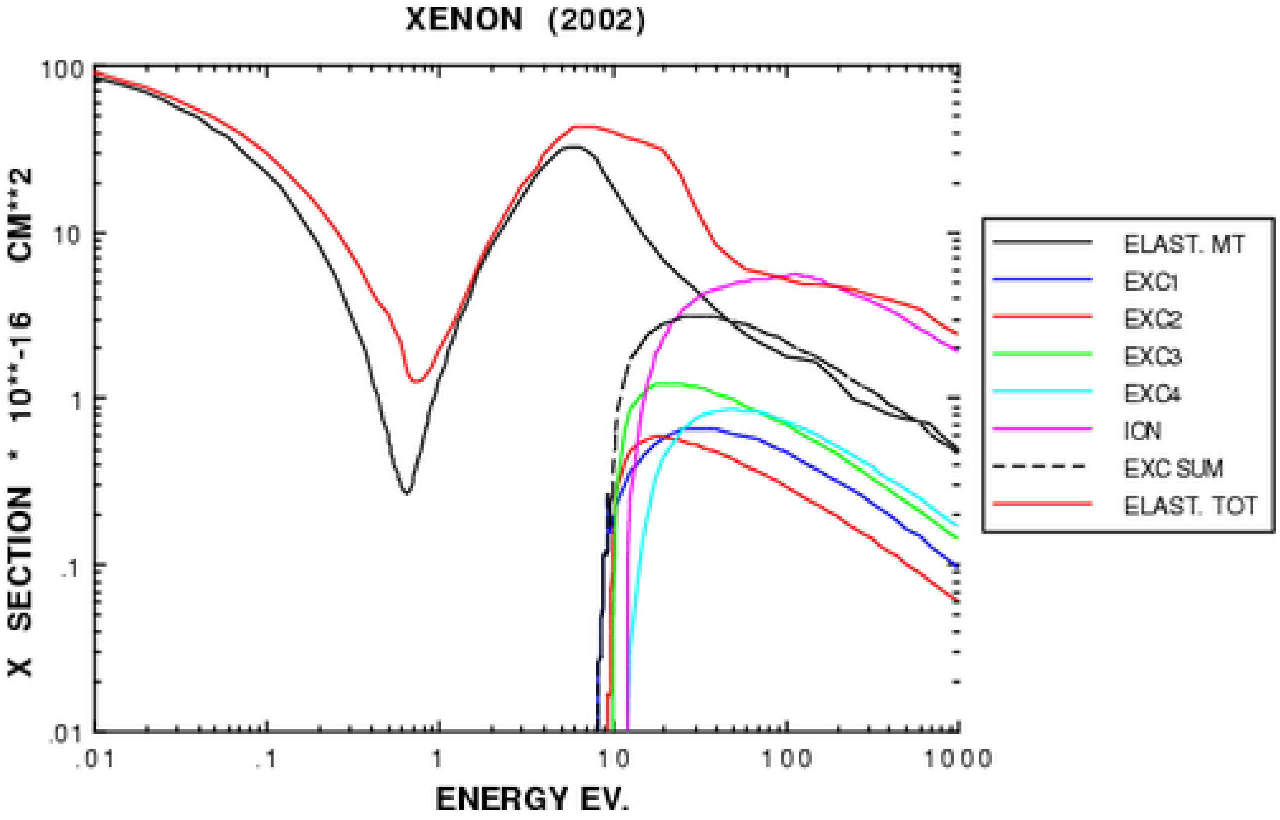
Resonance neutralization – forbidden transitions

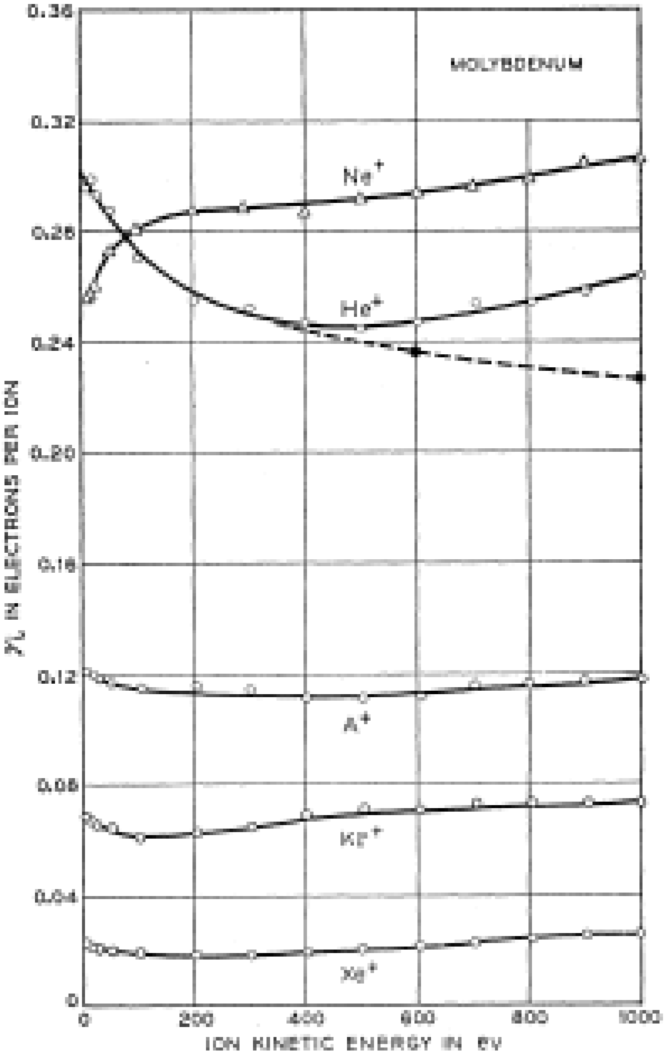


Ion ground state *above* bottom of valence band

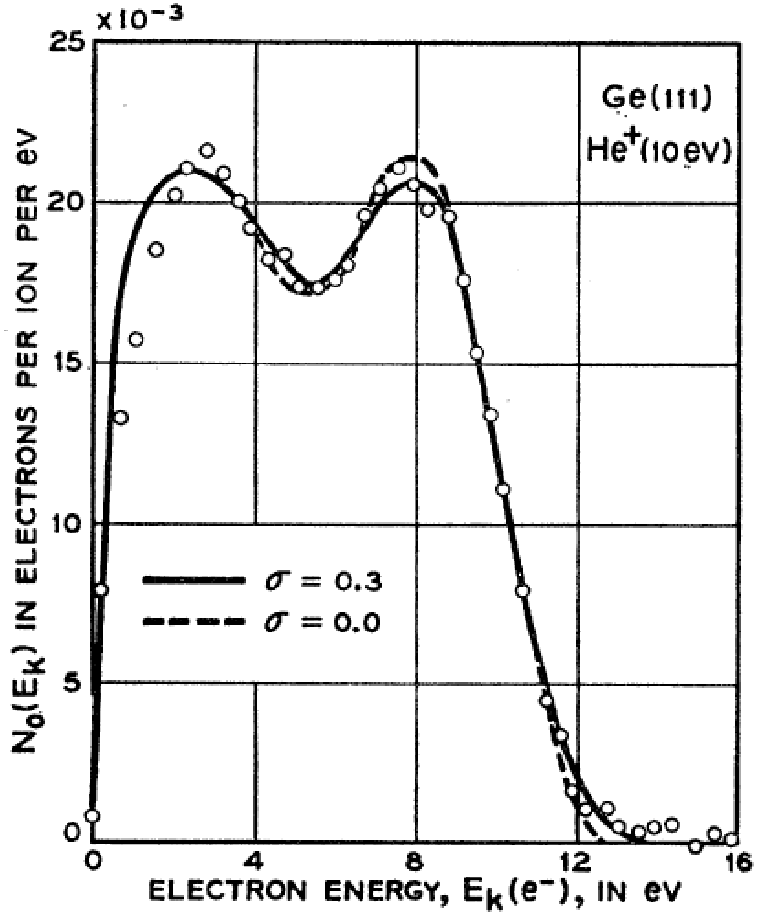
If the energy lost by electron 2 is smaller than the band gap the transition is forbidden and the excess energy is released by other mechanisms (e.g., photon emission).

Xe cross sections (Magboltz)



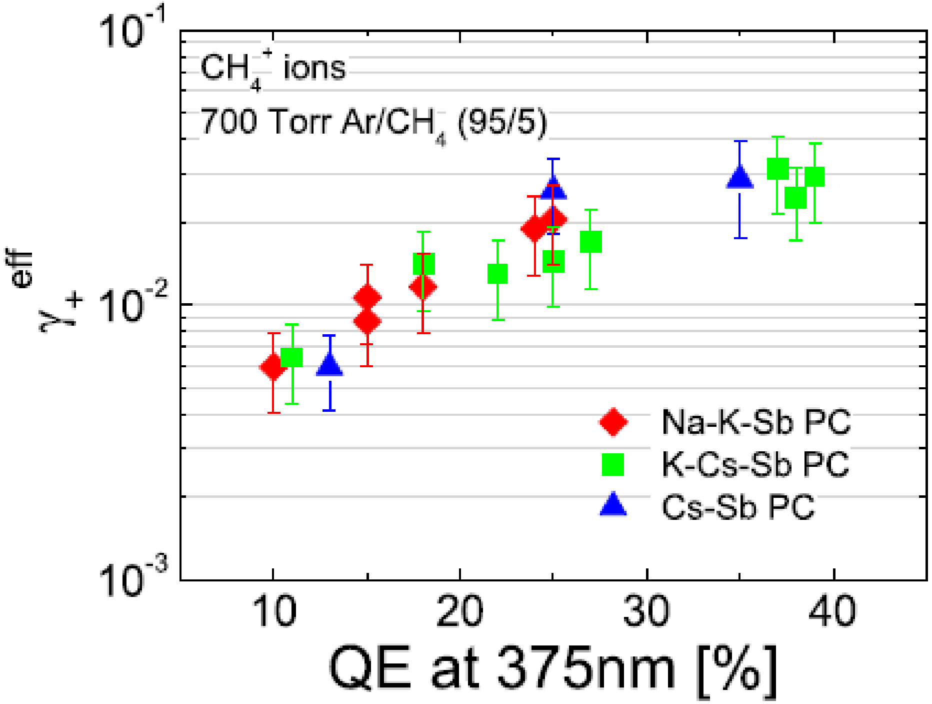


H. D. Hagstrum, Phys Rev 104 (1956) 672



H. D. Hagstrum, Phys Rev 122 (1961) 83

γ_i and γ_{eff} for CH_4 ions on bialkali photocathodes



$$\varepsilon_{ext} = 6\%$$

$$\gamma_i = 47 - 49\%$$

Lyashenko et al, J. Appl. Phys. 106 (2009) 044902