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QUALIFICATION ALTERNATIVES TO SPR

SAND2011-8327P

CASCADE III-V Capability and Results

QASPR Independent Review

November 9-11, 2011

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Department 1384

SAND2011-xxxx

NNSA National Nuclear Security Administration

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CASCADE Code

ROLE:

Using the Threat or Simulation Neutron Fluence, Time History and Energy Spectra – Generate the Early Time Displacement Damage Profiles in Semiconductor Materials of Interest

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Implementing New III-V Capability in CASCADE

- Implement Additional Empire Recoil Spectra Databases
  - In-113
  - In-115
  - P-31
  - Al-27
- Converge on a Threshold Displacement Energy for Marlowe for GaAs
  - MD Comparisons
- Pick Threshold Displacement Energies for InP and AlGaAs
  - ~ Literature Values

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CASCADE / NuGET QASPR Roles

- Production Code Path for Frenkle Pair production Rates – NuGET
- NuGET – Traditional ASC Code
- CASCADE – Physics / Model Development Code
  - Frenkle Pair Production – for use in NuGET
  - Defect Maps – for cluster analysis and device physics modeling work

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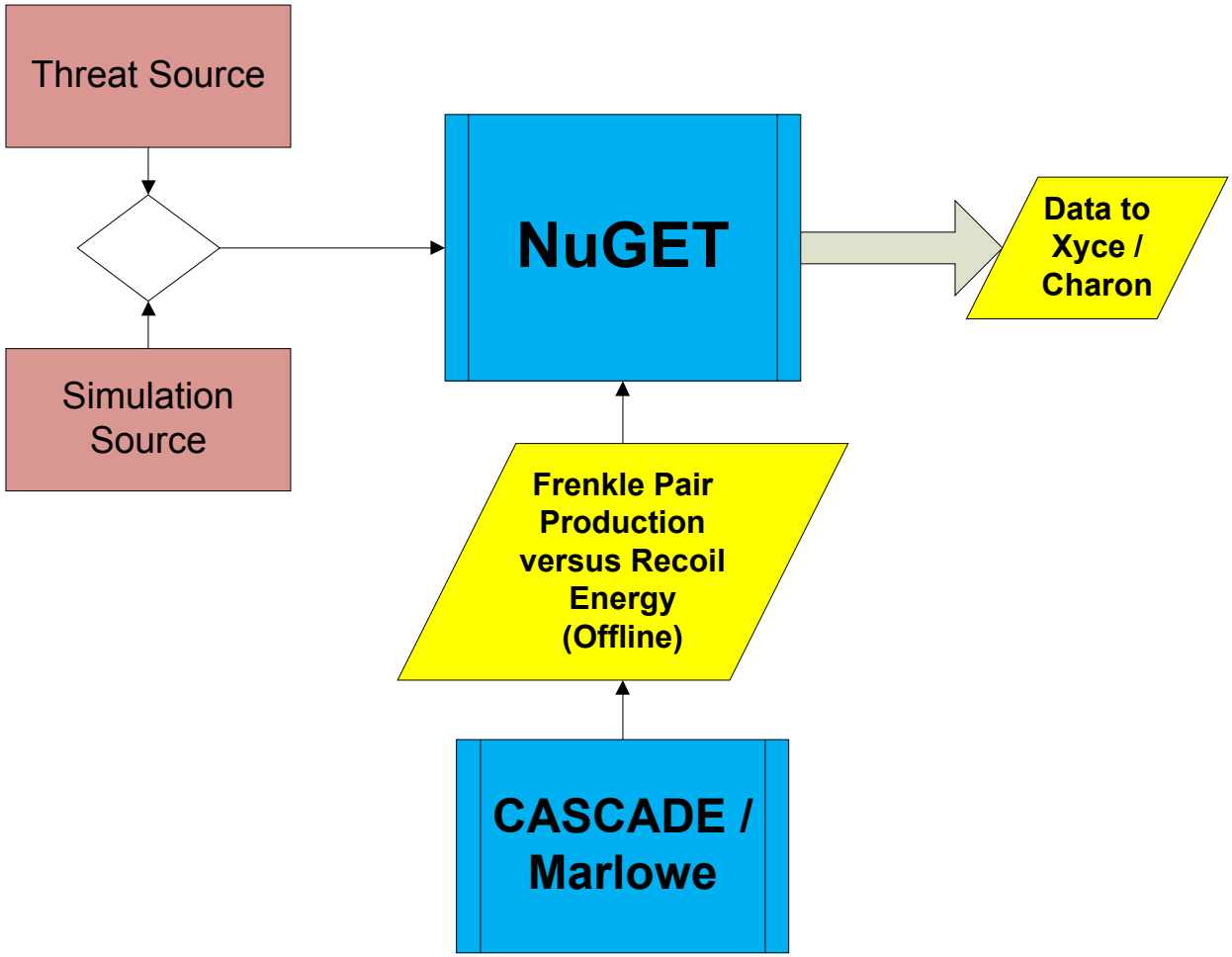
QASPR Production Flow



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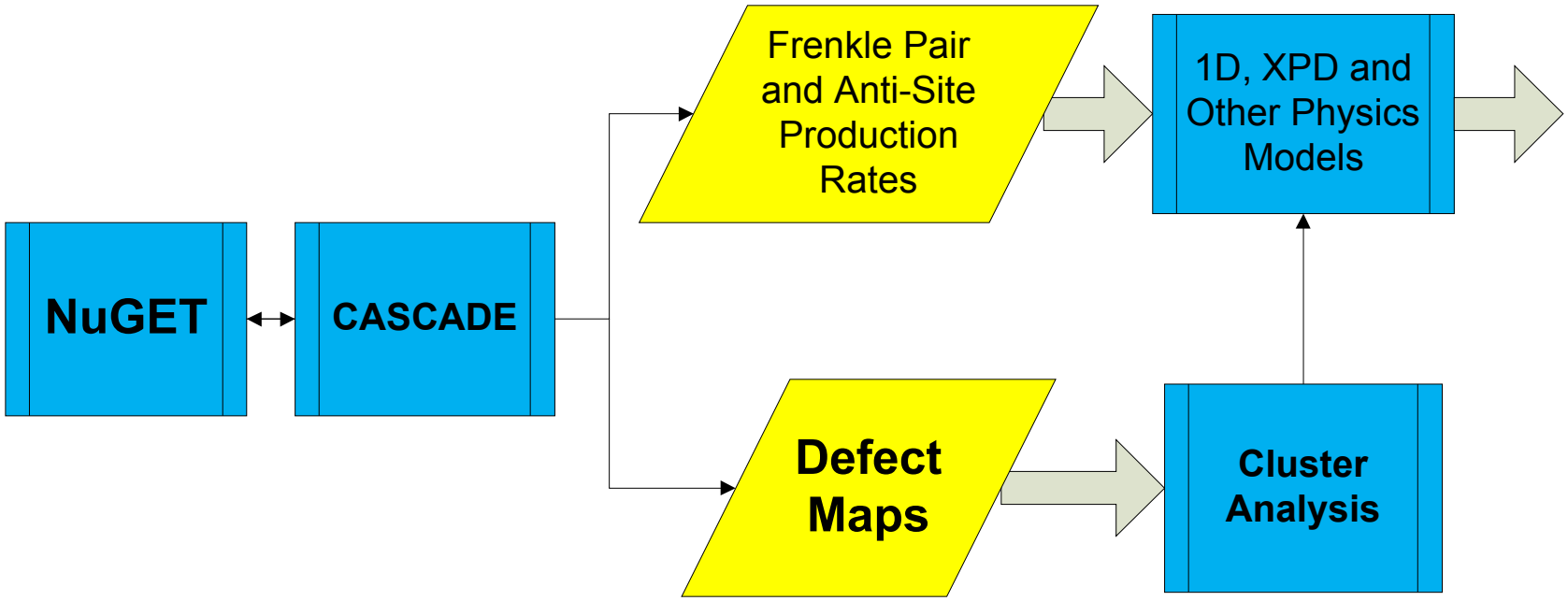
QASPR Model Development Flow



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The Ga and As results are very similar

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Si and GaAs CASCADE Results – Nov 2010

Facility	SPR		ACRR		
Environment	CC		PbB Bucket		
Lattice Material	Si	GaAs	Si	GaAs	
Recoil Model	EMPIRE	EMPIRE	EMPIRE	EMPIRE	
Quantity					**Units**
FP / Fluence	51.10	48.28	33.52	30.74	$(FP/cm^3) / (n/cm^2)$
Cascades / Fluence	0.1732	0.2106	0.1492	0.3624	$(Reactions/cm^3) / (n/cm^2)$
Avg No. FP per Casade	294.8	229.3	176.2	84.8	FP / cascade
Avg. Recoil Energy	54.56	18.25	39.61	6.67	keV

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III-V CASCADE Results – Oct. 2011

Facility	SPR		SPR		
Environment	CC		CC		
Lattice Material	Si	GaAs	InP	AlGaAs	
Recoil Model	EMPIRE	EMPIRE	EMPIRE	EMPIRE	
Quantity					**Units**
FP / Fluence	51.10	38.82	110.84	33.96	$(FP/cm^3) / (n/cm^2)$
Cascades / Fluence	0.1732	0.2106	0.1780	0.2119	$(Reactions/cm^3) / (n/cm^2)$
Avg No. FP per Casade	294.8	185.8	628.4	169.3	FP / cascade
Avg. Recoil Energy	54.56	18.21	45.9	19.0	keV

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Conclusions

- QASPR has a demonstrated III-V capability in CASCADE
- There are issues in determining the Threshold Displacement Energies for the new III-V Materials
- The Role of CASCADE is evolving in the QASPR Process

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Future Plans

- Comparisons of Frenkel Production for GaAs in CASCADE and NuGET
- Perform InGaP and InAlAs Calculations
- Marlowe Ion Beam Calculations supporting the Ion Beam experimental work
- Pair Correlation Function analysis in CASCADE
- Additional Recoil Spectra
  - Boron
  - Nitrogen

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