

Making digital twin work

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Short Bio

- Chair professor for Micro/nanoelectronics system integration and reliability, Delft University of Technology; IEEE Fellow; Secretary general of IEEE ITRW
- Philips Research Fellow until May 2013; NXP Senior Director for technology strategy until 2009



Outlines

- Motivation
- State-of-Art
 - Material modeling and characterization
 - Process design and modeling
 - Tests and Qualifications
 - Health monitoring and lifetime prognostics
- Challenges and Roadmap
- Summary



Autonomous driving



Source: www.ibeo-as.com

Intelligent manufacture



Source: www.ptc.com

Al for X Smart city ···· 84 000 **ŤU**Delft

Smart service



Source: www.jeanhillstudios.com

Source: mashdigi.com

Reliability: The major concern of high-tech industries

Warranty claims: 2% of global annual industrial revenue; delayed product release; liability; reduced consumer confidence





Business consequences

Warranty claims US companies

Company	2009 Accrual s in	2009 Claims Rate (% of sales)	2008 Claims Rate	2007 Claims Rate
	Mio \$		(% of sales)	(% of sales)
Lexmark International	84	9.0%	8.4%	13.0%
Garmin Ltd.	165	5.6%	3.8%	
Hewlett-Packard Co.	2,701	3.6%	3.7%	2.9%
Eastman Kodak	88	3.2%	1.9%	
Whirlpool Corp.	396	3.0%	2.8%	3.8%
Caterpillar Inc.	880	3.0%	2.6%	2.2%
IBM Corp.	374	2.3%	2.0%	2.8%
Dell Inc.	995	2.3%	2.0%	2.2%
Microsoft Corp.	148	2.1%	2.4%	6.2%
Black & Decker Corp.	92	1.9%	2.0%	1.8%
Ford Motor Co.	1,561	1.5%	1.7%	2.6%
Cisco Systems	381	1.5%	1.2%	
Motorola Inc.	301	1.4%	1.5%	2.0%
Harley-Davidson Inc.	51	1.3%	1.0%	1.2%
Apple Inc.	303	1.0%	0.9%	1.0%
General Electric Co.	780	1.0%	1.2%	0.8%
Johnson Controls	257	1.0%	0.8%	
Honeywell International	188	0.8%	0.8%	0.7%
Boeing Co.	167	0.5%	0.5%	0.7%



Source: SEC, via Warranty Week



Past solutions with handbooks

Since 1960s, several reliability prediction handbooks have been published, with applications in Aviations and Defenses, Telecommunications, Automotives, Electronics and Computers, and Mechanical Equipments.



Past solutions with empirical models

Arrhenius Model, Eyring Model, Voltage/Field Effect Model, Current Model, Power Model, Temperature Cycling Models, Humidity Models...







where MTF, median time to failure (hrs), A pre-factor constant, j current density (A/m²), ϕ activation energy (eV), k Boltzmann constant (J/K), T temperature (K)

Humidity driven failure models

Lawson model: $t_f = A \cdot e^{\Delta E/kT} e^{bRH^2}$ Eyring model: $t_f = A \cdot e^{\Delta E/kT} e^{B\cdot RH}$ Peck-Zierdt model: $t_f = A \cdot e^{[\Delta E/kT + B(nRH)]}$ Reich-Hakim model: $t_f = A e^{[\Delta E/kT + B(nRH)]}$ Weick model: $t_f = A \cdot e^{\Delta E/kT} \cdot e^{(B \cdot T/RH)} \cdot e^{(C \cdot RH)}$



ISPSD 2015, 385-388

where RH= relative humidity

- Need comprehensive knowledge of failures
- Can't consider the field's uncertainties and dynamics
- Require significant time and operation cost, experience based



Digital Twin for Mission Critical Electronics (MCE)

- MCE grows fast
- "Performance and lifetime on demand" becomes essential
- DT will be the key enabler







Digital Twin (DT) contains 3 main parts:

- Physical products/systems in Real Space, i.e. materials, products, processing, operation, recycle...
- Virtual products/systems in Virtual (digital) Space, i.e., simulation models.....
- Connectivity of data, information and instruction that connect the virtual and real worlds together



3 Connectivity Scenarios (combination is also possible)

Weak connection



- □ Modeling as a supporting tool
- No closed loop

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- □ Virtual prototyping
- □ Product and process design

Cloud connection



- Real-time monitoring/data filtering/transmission
- Cloud platform, complicated simulation models, cloud computing
- Output filtering, intelligent control
- Separated closed loop

Embedded connection



- Real-time monitoring/data filtering/transmission
- Highly reliable DT chip (or embedded in MCU), with built in simpler/compact models and edge computing
- Integrated close loop, control & decision-making

The Landscape of Digital Twin



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Material modeling and characterization: NanoCu

MD assisted Material design and modeling

• Anti-oxidation coating



Sintering mechanism
 Impact of P, T, t, etc.



• MEMS micro-hotplate based time-resolved in-situ SEM



MD assisted property characterization

Electromigration

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• Sulphidation



Oxidation



Material modeling and characterization: Cu/SiO₂ interface

Multiscale modeling from First principles simulation to molecular dynamics simulation to finite element modeling



Z Cui, X Chen, X Fan, GQ Zhang, Interfacial Properties of Cu/SiO2 using a Multiscale Modelling Approach in Electronic Packages, EuroSimE 2018. 15

Material modeling and characterization: Phosphors

Ab-initio/First principle modeling of hydrolysis mechanism for R6535 CaAlSiN₃:Eu²⁺ red phosphor



First principles simulation

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 $CaAlSiN_3(s) + 2H_2O(l) \rightarrow Ca^{2+} + 2OH^- + H_2AlSiN_3(s)$

Moisture driven degradation of CaAlSiN₃:Eu²⁺ red phosphor can be attributed to the **initially dissolved of Ca²⁺ and OH-**, gradually **crashed crystallinity of host lattice and the increased surface roughness** from reaction residues.

Material modeling and characterization: Phosphor/silicone interface

Ab-initio/First principle modeling of mechanical properties for Phosphor/silicone interface

(a)

fensile strength (MPa)



Pristine CaAlSiN₃[010] surface, the minimum-energy pathway along (a) [100] direction. (b) [001] direction.



Hydrolyzed CaAlSiN₃[010] surface, the minimum-energy pathway along (a) [100] direction. (b) [001] direction.

MD based low-k material/interface design

Motivations

- Develop/design reliable low-k
 material and interface
- Using molecular dynamics to model the nanoscale material and interface

Scientific challenges

- Modeling
- -Amorphous and porous material
- -Chemical bonding status at interface
- Experimental comparison



Approaches



Results

• Prediction of mechanical properties of low-k material



0.010 0.016

Applied Displacement (nm)

 Prediction of interfacial strength of low-k material



Molecular simulation strategy for mechanical modeling of amorphous/porous low-dielectric constant materials. <u>Appl. Phys. Lett</u>. 92, 2008 Example: Molecular dynamics analysis for multi-scale reliability assessment of CNTs



Problem

 Mechanical stability of CNTs will affect the reliability and performance

Scientific challenge

 Computational studies overcome the limitations of experimental approaches and give extra control on parameters such as defect position

Results

- Defects near the deflection points of the CNT, reduce the critical buckling load (about 70%) at low temperature
- ^tDefects do not significantly alter the critical buckling load at room temperature

Effects of single vacancy defect position on the stability of carbon nanotubes, **Journal of Microelectronics Reliability, 52, (2012)**

Material modeling and characterization: CNT pillars

Multiscale modeling of failure modes for CNT pillar with and without a-SiC coating





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Material modeling and characterization: WS₂ sensor Effects of Defect and Temperature on the Mechanical

Performance of WS₂: A Multiscale modeling



Material modeling and characterization: Electromigration



$$Z^* e \rho j + \Omega \frac{\partial \sigma}{\partial x} = 0$$

$$jL = \frac{(\sigma_{max} - \sigma_{min})\Omega}{Z^* e \rho}$$

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Electromigration measurement

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Electromigration Electron Wind Stress-migration Self-diffusion Concentration Gradient Stress Gradient Atomic Transport Temperature Gradient Thermomigration $\left(\frac{2EA\Omega f}{9(1-\nu)k_BT}\right)\frac{\partial^2 C_{\nu}}{\partial x^2} + \frac{Z^* e\rho j}{k_BT}\frac{\partial C_{\nu}}{\partial x} =$ $\frac{\partial^2 C_v}{\partial x^2} + \frac{Z^* e\rho j}{k_B T} \frac{\partial C_v}{\partial x} = 0$

Cui Z. Fan X. J. Zhang G.Q. et al., J. Appl. Phys., 2019

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Physics of Failure (PoF) Based Reliability Modeling



Process design and modeling: Reflow process

A Moisture-Thermal-Mechanical coupling modeling of moisture-induced stresses of IC packaging during reflow process



- Fan XJ, Moisture sensitivity of plastic packages of IC devices, Springer, 2010.
- Chen L et al., Microelectronics Reliability, Vol. 75, 2017, pp. 162-170.
- Chen L et al., Appl. Mech. Rev., 70(2), 2018, pp. 020803
- Ma L et al, 2019 IEEE 69th, 2019, pp. 806-810.
- Chen L et al., 2020 ECTC.

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Process design and modeling: Sintering process

Molecular dynamics simulation: Pressure-assisted NanoCu sintering



Dong Hu, Zhen Cui G.Q. Zhang et al., Results in Physics, 2020

Process characterization: MEMS enabled time-resolved X-ray diffraction for NanoCu sintering



Process design and modeling: FC packaging process



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Yuan C and Lee C.C., 2020 21th EuroSimE Yuan C et al, 2019, 20th EuroSimE

Liu W et al, 2020 70th ECTC Chou P et al, 2019 69th ECTC

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Process design and modeling: SiC MOSFET module

Fan-Out Panel-Level SiC MOSFET Power Module

Ant Colony Optimization-Back Propagation Neural Network





 Y_1

Y_m

Output layer

Hidden laver





Thermal optimization





Thermal-Stress optimization

	After RSM	After ACO- BPNN	Before optimization	Percentage improvement by RSM	Percentage improvement by ACO- BPNN
Temperature T (°C)	180.71	180.40	187.02	3.38%	3.50%
Stress σ (MPa)	24.453	24.728	27.490	11.05%	10.04%

Y. Qian, F. Hou, J. Fan, Q. Lv, X. Fan and G. Zhang, *IEEE Transactions on Electron Devices*, doi: 10.1109/TED.2021.3077209. 28

Process design and modeling: Chip/Package/System Co-Design





Capped-Die Flip Chip Package

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- Warpage-free packaging with a capped-die flip chip package co-design (cap/board thickness, underfill property...).
- WLP placement/secondary component at system level.



Shen Y et al., IEEE Transactions on CPMT 6(9), 1308 – 1316. 2016 Fan XJ et al., IEEE Transactions on CPMT. 2(11), 1802-1810, 2012... No secondary

component

Scenario I

Scenario 2

Right-side ball

BGA outline

U8

Left-side ball

Example: CMOS 90/65nm IC/packaging co-design

Problem & Challenges

Multi-physics; multi-failure mode; non-linear & time dependent; simulation-based optimization



Objective

Develop IC/package co-design tool that can ensure the thermomechanical reliability, as the functions of waferfab backend process and packaging design parameters

Methods







Heterogeneous Integration Roadmap Workshop

Moving towards a new paradigm



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<u>Cost effective testing strategy and test methodologies;</u>
 <u>Automated test pattern generation, data analysis and diagnosis flows;</u>
 <u>Multifunctional performance testing;</u>
 <u>Multi-scale testing;</u>
 <u>Multi domain cross talk;</u>
 <u>Complex system testing.</u>

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Accelerated Test Method of Luminous Flux Depreciation for LED Luminaires and Lamps



An accelerated test method for luminous flux depreciation to reduce the test time from 6000 to 2000 hours at an elevated temperature

Accelerated Tests of Remote Phosphor: PC+ YAG:Ce

- Remote phosphor: PC+ YAG:Ce
- Ageing at 80, 100, and 120 °C for 3000 h
- Light intensity of: 825, 3300,13200 W/m²





Light intensity (W/m2)	825	3300	13200
Temperature (°C)			
80	4410	4370	4300
100	4120	4000	3900
120	4050	3900	3720

Maryam Yazdan Mehr; van Driel, WD; GuoQi Zhang; Microelectronics Reliability, Volume 54, Issue 8, pp. 1544-1548, 2014.

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Color Shift-high temperature accelerated ageing tests of LED diffuser/Lens



Inconsistent degradation of wavelength-dependent transmittance

Lu GJ, Mehr MY, van Driel WD, Fan XJ, Fan JJ, Jansen KMB, and Zhang GQ, Optical Materials. vol. 45, pp. 37–41, 2015.

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Health monitoring and Lifetime Prognostics: Fusion method



A Prisacaru, PhD dissertation, TU Delft, 2021

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Al assisted Simulation & Design



AI assisted new material design



Lifetime Prognostics: PoF method for LEDs



B. Sun, X.J. Fan, G.Q. Zhang et al., IEEE TRANSACTIONS ON INDUSTRIAL ELECTRONICS, 2016 41

Lifetime Prognostics: Data-driven method for LEDs



Bayesian method (BM)

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- The exponential decay model is used as the degradation model and the parameters are estimated based on Markov Chain Monte Carlo (MCMC) sampling and using the Metropolis-Hasting (MH) algorithm.
- The lifetime prediction results showed that the Bayesian method has better prediction accuracy compared to the NLS method.

Metamodel based AI using Adaptive DOE

- A machine learning technique that aims to provide the best metamodel fitting capability given a certain design space.
- An **iterative approach** that learn and focus on the most interesting regions for the creation of a better metamodel.
- A flexible methodology that smoothly scales from single output to multi-output problems
- A powerful technique that avoids undersampling and/or oversampling issues.

Reuse re	Adaptive DO	DE Options	
Reject	Random seed	28	
rpe Adapt	Maximum number of evaluations	50	= 50
Inputs Ou	Learning population size	5	
	Strategy	Full Exploration	6
	Model type	RBF	-
On	Accuracy	1	
1 🖌	Output Guarantee	v	= 10
2 🗸	Use start point	•	= 13
	Start population	No method selected \checkmark	
	Default	values	
	OK	Cancel Help	
	OK	Apply Cancel	Help





Multiscale & Multiphysics modeling







HIR Simulation/modeling chapter

Question:

"We developed a new product/system, by using new materials and new technology, can you tell when will it fail and how? "

My answer is NO.



- In principle, all simulation results are wrong, unless you can prove they are right
- Experiments (characterization and verification) will remain as the key success factor for simulations and modeling
- Easier to develop sophisticated simulation models, than to build a simple ones
- It is easier to make ones' models beautiful than useful. But, nice pictures will not make your boss happy. The ultimate aim is to achieve "Design on Demand" - SOLUTIONS
- Key mission of simulation community: to liberate the simulation experts by combined data, physics of failure based models with AI/ML.

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Physical twin challenges:

- Rapid prototype
- First-time-right design
- Optimized performance & designed in reliability
- Low cost and reliable sensing and in-situ monitoring
- Self healing

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- Remaining useful life prediction
- Proactive maintenance
- C2C and lifecycle optimization

Optimum ost (unit Failure Maintenance Health Index Maintenance time rediction Reliability current time Te: designed 5-10 yrs DT chip/function integrated 3-5 yrs • Performance and lifetime Sensing and in-situ monitoring on demand Accurate fault alarm ٠ D4X Remaining useful life ٠ ٠ Current Rapid prototype First-time-right design ٠

• Optimized performance

Digital twin challenges:

- Accurate and efficient simulation models
- Nonlinear, time and temp dependent
- Fast and accurate multi-scale/multi-physics/fullprocess simulations
- From deterministic to probabilistic/stochastic simulation
- Accurate failure threshold definition
- Multi-failure modes interaction & solution
- Automated model generation and simulation
- Compact models
- Integration of physics of failure based models with ML and data driving models
- Simulation based optimization/design& operating rule

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- Analytical/empirical models 1st principle/MD quantitative
- FEA modeling for known failure modes
- Trial-and-Error

Current

3-5 yrs

- Integrated multiscale/multiphysics
- simulations
- **Optimisation & design** rules
 - AI assisted & data driven simulation and design
- Design for reliability

5-10 yrs

- Multi-scale/multi-physics/fullprocess simulations
- Nonlinear, dynamic, probabilistic ٠ /stochastic simulation
- AI/data driven automated • simulation models
- Design 4 X
- Upgradeability

Connectivity challenges:

- Cloud platform and connection
- Low cost and reliable real-time monitoring
- Big data storage, transmission, smart filtering, computing, close loop control algorithm
- Smart sensing and IoT wireless communication
- Highly reliable embedded DT chip/MCU integration
- ...

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3-5 yrs

- Cloud platform
- Real-time key parameter monitoring
- Big data storage, filtering, transmission and computing
- IoT wireless communication
 - Separated closed loop

5-10 yrs

- Smart in-situ sensing and transmission
- Edge computing
- Highly reliable embedded DT chip/integrated with MCU

Current

- Weak connection
- No closed loop
- Limited data of in-situ

monitoring



Lifetime Prediction Digital Twin System : Structure of Data Flow and Processing

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Summary

- Driven by the ever-increasing societal needs for digitalization and intelligence, such as autonomous driving, Manufacture 4.0, "Smart-X", "AI in all", the demands for mission critical electronics components and systems are growing fast.
- To realize "performance and lifetime on demand" for mission critical electronics, DT will play an essential role.
- The DT must be able to represent the PT reliably and efficiently, to achieve the ultimate aim of 1+1>2.





- From analytical, empirical and numerical to NOVEL methods, evolutionary / revolutionary modeling& simulation ideas are not mature yet.
- Integrated & concurrent development of physics of failure based models with AI driven big data/ML are possible solutions to predict the multi-scale/multiphysics/full process/nonlinear/stochastic/time and temperature dependent responses of mission critical electronics.



Thanks for your attention DIGITAL **ŤU**Delft