MODELING OF TRAPPING/DETRAPPING OF HYDROGEN ISOTOPES IN TUNGSTEN MATERIALS

WHISCI modeling TEAM
(CS Becquart, R Bisson, N Fernandez, Y Ferro, C. Grisolia, E. Hodille, J Mougenot)
TORE SUPRA going WEST

CIEL configuration

WEST configuration
WEST Plasma Facing Components: full metallic actively cooled environment

- Upper target: Water-cooled Stainless steel panel, W-coating
- Ripple/VDE protection: W-coating
- Water cooled Stainless steel panel
- Bumper: W-coating
- Lower target: ITER Divertor Technology
- Baffle: W-coating
- Antenna Limiters: B-coating (W?)

**ITER requirement:**
- *10 MW/m² in steady state*
- *20 MW/m² in slow transient (< 10s)*
WEST plasma scenarios

- **H1**: testing ITER PFC
  Long pulse 10-20 MW/m²

- **H3**: high fluence
  ITER fluence in a few days of operation

- **H4**: high power
  Shorter pulse towards hybrid scenarios

<table>
<thead>
<tr>
<th>SCENARIO (3.7 T)</th>
<th>HIGH POWER</th>
<th>STANDARD</th>
<th>HIGH FLUENCE</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>H4</td>
<td>H1</td>
<td>H3</td>
</tr>
<tr>
<td>Plasma current</td>
<td>0.8 MA</td>
<td>0.6 MA</td>
<td>0.5 MA</td>
</tr>
<tr>
<td>Plasma density</td>
<td>$9 \times 10^{19}$ m⁻³</td>
<td>$6 \times 10^{19}$ m⁻³</td>
<td>$4 \times 10^{19}$ m⁻³</td>
</tr>
<tr>
<td>Total radiofrequency heating power</td>
<td><strong>15 MW</strong></td>
<td>12 MW</td>
<td>10 MW</td>
</tr>
<tr>
<td>Lower Hybrid Current Drive</td>
<td>6 MW</td>
<td>6 MW</td>
<td>7 MW</td>
</tr>
<tr>
<td>Ion Cyclotron Resonance Heating</td>
<td>9 MW</td>
<td>6 MW</td>
<td>3 MW</td>
</tr>
<tr>
<td>Plasma current flat-top duration</td>
<td>30 s</td>
<td>60 s</td>
<td><strong>1000 s</strong></td>
</tr>
<tr>
<td>Expected heat load*</td>
<td>10 MW/m²</td>
<td><strong>10-20 MW/m²</strong></td>
<td>10-20 MW/m²</td>
</tr>
<tr>
<td>Expected ELM frequency</td>
<td>59 Hz</td>
<td>76 Hz</td>
<td>77 Hz</td>
</tr>
<tr>
<td>Expected ELM load</td>
<td>40 kJ/m²</td>
<td>52 kJ/m²</td>
<td>74 kJ/m²</td>
</tr>
<tr>
<td>Expected operation time to reach one ITER pulse particle fluence</td>
<td>~6 months</td>
<td>~2 months</td>
<td>~few days</td>
</tr>
</tbody>
</table>

**H2**: long pulse H mode
Pre-requisite for the programme

Ion flux: $10^{22}$ $10^{23}$ D/s m²
CRP VIENNA 2013, PROPOSED APPROACH

- ab initio, dft
- Molecular dynamics
  - (10 nm), ns
- Binary collision approximation

Multiscale Modeling

- Finite elements
- Micro-macro

- Dislocation dynamics
- Phase Field
- Rate Equations
- Okmc

+ crosscheck with experimental data

THE WHISCI PROJECT: W/H INTERACTION STUDIES IN A COMPLETE AND INTEGRATED APPROACH

WHISCI – Predict and control Tritium/Deuterium trapping/degasing

Real/Complexity

Models
- macroscopic
  « Rate Equations (RE)
  + Finite Element Methods (FME) »
- mesoscopic
  « Object Kinetic Monte Carlo (OKMC) »
- microscopic
  « Density Functional Theory (DFT) »

Experiments
- Realistic wall
  « ITER-WEST grade »
- Semi-realistic wall
  « polycrystals (controlled defects) »
- Model wall
  « single crystals (controlled defects) »

Multi-scale modeling validated by well controlled laboratory experiments

Coordinator: Regis Bisson (PIIM Laboratory)
THE WHISCI PROJECT:
W/H INTERACTION STUDIES IN A COMPLETE AND INTEGRATED APPROACH

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Strong and constant interactions in place
(starting 3 years ago)
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DFT results presented here are deeply detailed in:


Small number of atoms (54 atoms)

Pure Single Crystal (where vacancies can be introduced)

Up to now, no surface effects (implementation in progress)
DFT: H TRAPPING IN VACANCIES

H interstitial as solute

Multi-trapping

Vacancies

Up to 12 H atoms in a vacancy
Using kinetic modeling, it can also be shown that during a Thermo-desorption experiment:

**Desorption T at peak maximum**

<table>
<thead>
<tr>
<th>$\beta = 1, \text{K}\cdot\text{s}^{-1}$</th>
<th>6H</th>
<th>5H</th>
<th>4H</th>
<th>3H</th>
<th>2H</th>
<th>1H</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{\text{des}}$ (eV)</td>
<td>0.86</td>
<td>1.11</td>
<td>1.17</td>
<td>1.25</td>
<td>1.42</td>
<td>1.43</td>
</tr>
<tr>
<td>$T_{\text{max}}$ (K)</td>
<td>311</td>
<td>399</td>
<td>420</td>
<td>447</td>
<td>507</td>
<td>511</td>
</tr>
</tbody>
</table>

**Filling level at RT:** VH6
Perfect crystal submitted to a H flux up to H concentration: $10^{-5} (\equiv 10^{22} \text{ D m}^2/\text{s})$ ⇒ $VH_j$ fractions at Thermo Equilibrium

- $300K < T < 550K$ – $VH_6$
- $550K < T < 1000K$ – pop. Inverted
- $T > 1000K$ – vacancies depopulated
Simple kinetic model:

- diffusion is neglected (0.2eV)
- the surface of the sample is neglected
- hydrogen is assumed to desorbed as released from a vacancy type VH_j
- kinetics of order one are assumed

TDS conditions:

- H implantation T=300K
- VH_j fraction from stat. model
- \( \beta = 5 \text{Ks}^{-1} \)
- \( 0.85 \times 10^{13} \text{ Hz} < \nu < 1.45 \times 10^{13} \text{ Hz} \)
DFT: MODELLING THERMO-DESORPTION WITH A CRUDE MODEL

Low temperature peaks

VH3-5
T=420K

High temperature peaks

VH1,2
T=540K

TDS peaks include desorption from multiple VH$_j$ traps

Exp.

VH6
Not observed
Already desorbed

VH3-5
T=420K

VH1,2
T=540K

Run #11
no LN$_2$ cooling
5.5 K/s to 1750 K

Run #13
no LN$_2$ cooling
5.2 K/s to 1750 K

Run #19
no LN$_2$ cooling
5.8 K/s to 1265 K

Run #12
with LN$_2$ cooling
6.4 K/s to 1700 K

Run #15
with LN$_2$ cooling
5.1 K/s to 1710 K

Run #16
with LN$_2$ cooling
5.0 K/s to 1780 K
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Object Kinetic Monte Carlo

Microstructure = objects defined by:
- type
- centre-of-mass position
- reaction radius
- possible reactions

PBC : periodic boundary conditions

Large box: 330nm of depth (see end of presentation)
Object Kinetic Monte Carlo

Microstructure = objects defined by:
- type
- centre-of-mass position
- reaction radius
- possible reactions

Internal events: migration of the objects, emission from the objects or capture
External events: H / He implantation, neutron irradiation…
Object Kinetic Monte Carlo

Microstructure = objects defined by:
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External events: H / He implantation, neutron irradiation...

Objects that we can encounter in the OKMC box:
- vacancies, interstitials, impurities, dislocations, grain boundaries, helium atoms, ...
- If they can form clusters, these clusters are a different object: i.e. a cluster which contains 3 vacancies and one H atom is an object.
What can we obtain?
A description of the microstructure in terms of positions of the objects in the volume and concentration

So we can model a desorption experiment for instance
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A description of the microstructure in terms of positions of the objects in the volume and concentration

So we can model a desorption experiment for instance

For all the objects that can move, we need their diffusion coefficient:

activation energy/migration barrier : $E_{\text{mig}}$

How can we obtain them?

- $E_{\text{mig}}$ from DFT, from experimental results, ... tuning parameters adjusted on experimental data one this is possible. So we need the diffusion coefficient of the mono-vacancy, the di-vacancy, the tri-vacancy and so on ......
What can we obtain?
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For all the objects that can emit:

- a di-vacancy can emit a vacancy, a tri-vacancy containing 2 hydrogen atoms can emit either a vacancy or an hydrogen atom, a grain boundary can trap an interstitial or an hydrogen atom and re-emit it, etc...

we need the binding energy of the emitted species with the object.

How can we obtain them?

From DFT for small objects, from experimental results, ... tuning parameters adjusted on experimental data one this is possible
OKMC is a tool that can be used to « check » the data obtained from DFT. For instance if DFT predicts that H migration energy is XXX eV, we plug this value into OKMC and see whether H desorption takes place at the right temperature …

I will come back to code comparaison at the end of this presentation
THE WHISCI PROJECT: W/H INTERACTION STUDIES IN A COMPLETE AND INTEGRATED APPROACH

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MACROSCOPIC RATE EQUATION (MRE) APPROACHES

- Usual one
  - developed to fit experimental data coming from polycrystal experimental studies
  - Check parameters, … without any link with physical processes
  - Approach is an “engineer” one

MHIMS code
(Migration of Hydrogen Isotopes in Metals)

- New one
  - Linked to the DFT approach
    - Used to integrated the DFT outcomes
  - Up to now, fit single crystal experimental data

MHIMS-reservoir
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MHIMS-reservoir
USUAL MRE APPROACH

Energy diagram of HIs in tungsten (W)

- $E_S$ = solubility activation energy
- $E_D$ = Diffusion activation energy
- $E_{T,i} = E_{B,i} + E_D$ detrapping activation energy. Trap = vacancies, grain boundaries ...
- $E_R$ = recombination activation energy

One trap of $E_B$ trapping energy contents one H atom
Energy diagram of HIs in tungsten (W)

Concentration and types of traps (from IBA)

- **Induced traps**
  - In stopping zone: high concentration, due to collisions
  - Up to 1µm, relatively high concentration due plastic deformations, vacancies diffusion,…

- **Intrinsic traps**
  - In the bulk, Low concentration
USUAL MRE: MODEL DESCRIPTION

MRE 1D modeling

\[
\frac{\partial C_{t,i}}{\partial t} = -C_{t,i} \cdot v_i(T) + v_m(T) \cdot C_m \cdot \left(1 - \frac{C_{t,i}}{n_i}\right)
\]

\[
\frac{\partial C_m}{\partial t} = D(T) \cdot \frac{\partial^2 C_m}{\partial x^2} - \sum \frac{\partial C_{t,i}}{\partial t} + S_{ext}
\]

- **\( n_i \):** trap density (intrinsic and created by incident ions)
- **\( D(T) \):** diffusion coefficient (m²/s)
- **\( v_i(T) \):** detrapping attempt frequency \( v_0 = 10^{13} \, s^{-1} \)
- **\( v_m(T) \):** trapping attempt frequency. \( v_m \propto D(T) \cdot n_i \)
- **\( S_{ext} \):** particles source by implantation
  \[
  S_{ext} = (1 - r) \cdot \varphi \cdot f(x)
  \]
  - \( r \): reflexion coefficient of HI on W, \( f(x) \): ions stopping range (both given by TRIM)
  - \( \varphi \): incident ion flux
Boundary conditions

- Desorption no limited by recombination:

\[ C_m(x = 0, L) = 0 \]

Experimental evidence of a desorption non limited by recombination

[1, 2]

Boundary conditions

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Experimental evidence of a desorption non limited by recombination

[1, 2]


TDS simulation in 3 phases

- Implantation (initially empty): \( T_{\text{imp}}, E_{\text{imp}}, \varphi \)
- “resting” phase: \( T_{\text{rest}}, t_{\text{rest}} \)
- TDS phase: \( T(t) = T_{\text{rest}} + \beta \cdot t \) \( \beta \): heating ramp (K/s)

MHIMS Code
(Migration of Hydrogen Isotopes in Metals)

FIT OF EXPERIMENTAL DATA WITH THE MIHMS MODEL

Fit of experimental TDS data

**Input implantation and TDS parameters:**
- \( E_{imp} = 200 \text{ eV/D (} r = 0.56) \),
- \( \varphi = 2.5 \times 10^{19} \text{ D.m}^{-2}.\text{s}^{-1} \),
- \( T_{imp} = T_{rest} = 300 \text{ K} \),
- \( \text{fluence} = 10^{22} \text{ D.m}^{-2} \),
- \( t_{rest} = 50 \text{ s} \),
- \( \beta = 8 \text{ K/s} \).

**Input trapping parameters with \( \nu_0 = 10^{13} \text{ s}^{-1} \):**
- Trap 1 (intrinsic): \( E_{T,1} = 0.87 \text{ eV (0.85)}, n_1 = 1 \times 10^{-3} \)
- Trap 2 (intrinsic): \( E_{T,2} = 1.00 \text{ eV, } n_2 = 4 \times 10^{-4} \)
- Trap 3 (extrinsic): \( E_{T,3} = 1.5 \text{ eV (1.45)} n_{3\text{max}} = 2 \times 10^{-2} \)
  Irradiation induced trap (\( \propto \text{fluence} \))

Retention versus fluence at 2 implantation temperatures

FIT OF EXPERIMENTAL DATA WITH THE MIHMS MODEL

At 300 K: Retention ~ fluence$^{0.5}$ => diffusion limited
At 500 K: Retention ~ fluence$^{0.7}$ => trap creation limited

[2]: Tian, JNM, 2010
[3]: Ogorodnokiva, JNM 2003
Effect of the duration of the “resting” phase on retention

Implantation at 300 K (fluence = \(10^{22} \text{ D.m}^{-2}\text{s}^{-1}\)):
“resting” time varying from 50 s to 300 000 s (83 h)

**FIT OF EXPERIMENTAL DATA WITH THE MIHMS MODEL**

45 % of initial inventory lost in ~ 80 h (confirmed by experimental observations)

D twice deeper in the bulk

TDS spectra peak apparently shifted to high temperature
Evolution of retention with the sample temperature during ions implantation

- $10^{23}$ D/m² - 200 eV/D - PCW - [2]
- $10^{23}$ D/m² - 200 eV/D - PCW - [4]
- $10^{24}$ D/m² - 500 eV/D - PCW - [5]
- Simu. - $10^{22}$ D/m² - 200 eV/D ($t_{rest} = 300 000$ s)
FIT OF EXPERIMENTAL DATA WITH THE MIHMS MODEL

- MHIMS model fits well the experimental data (PCW)
- No information of the fundamental trapping processes (just an engineer approach)
- This MHIMS code is in a crosschecked process using a test case to be fitted (Eurofusion approach) with two other codes:
  - HIIPC from LSPM, Paris
  - Klaus Schmidt code, Garching

  Good agreement observed
MACROSCOPIC RATE EQUATION (MRE) APPROACHES

- Usual one
  - developed to fit experimental data coming from polycrystal experimental studies
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MHIMS-reservoir
NEW APPROACH OF MACROSCOPIC RATE MODEL

MRE 1D modeling

\[
\frac{\partial c_{t,i}}{\partial t} = -c_{t,i} \cdot \nu_i(T) + \nu_m(T) \cdot c_m \cdot \left( 1 - \frac{c_{t,i}}{n_i} \right)
\]

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\frac{\partial c_m}{\partial t} = D(T) \cdot \frac{\partial^2 c_m}{\partial x^2} - \sum \frac{\partial c_{t,i}}{\partial t} + S_{ext}
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- trap 3 (extrinsic): \( E_{T,3} = 1.5 \text{ eV} \) \((1.45)\) \( n_3 = \text{variable concentration} \)

Each trap containing one HIs

Different from DFT outcomes
From DFT, one vacancy can contain at RT up to 6 HIs
Formalism

One single trap type (density $N_t$) can contain up to $n$ HIs

- **i-trap type**, $N_i = \text{density of } i\text{-trap filled with } 0 \leq i \leq n \text{ HIs}$,
  - $N_t = \sum_{i=0}^{n} N_i$
- $C_{t,i} = \text{concentration of particle in } i\text{-trap trap} = i \cdot N_i$
NEW APPROACH OF MACROSCOPIC RATE MODEL

**Formalism**

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- $C_{t,i} = \text{concentration of particle in } i\text{-trap trap} = i \cdot N_i$

**Mechanisms & equations**

$i$-trap type can be change into:

- $i+1$-trap type by trapping a solute particle
- $i-1$-trap type by detrapping of a trapped particle from that trap

For $0 < i < n$, \[ \frac{\partial N_i}{\partial t} = -\nu_m \cdot C_m \cdot N_i + \nu_m \cdot C_m \cdot N_{i-1} - \nu_i \cdot N_i + \nu_{i+1} \cdot N_{i+1} \]

And the mobile population is governed by:

\[ \frac{\partial C_m}{\partial t} = D(T) \cdot \frac{\partial^2 C_m}{\partial x^2} + \sum_{i=1}^{n} \frac{\partial C_{t,i}}{\partial t} + S_{ext} \]

**Code MHIMS-reservoir**

“Study of a multi trapping macroscopic rate equation model for hydrogen isotopes in tungsten materials”, E Hodille et al, accepted for publication, Physica Scripta, 2015
Boundary condition
- Desorption no limited by recombination:
  \[ C_m(x = 0, L) = 0 \]

No Trap Creation

Trapping input
- Up to 6 atoms in a single vacancy at room temperature

TDS simulation in 3 phases
Trapping in vacancy => **Single crystal tungsten (SCW)**

- Few data
  - Poon et al., JNM 2002:
    - fluence = $10^{21-22}$ D/m², flux = $10^{18}$ D/m²/s, 500 eV/D
    - Resting time ~ 8h – 72h + backing at 400 K during 1h30 min
    - Heating ramp = 4-6 K/s

- Quastel et al, JNM 2006: (2)
  - fluence = $10^{23}$ D/m², flux = $10^{20}$ D/m²/s, 500 eV/D
  - well controlled resting time and backing
  - Heating ramp = 5,5 K/s

- Poon et al.: low flux and low fluence => **trap creation neglected** but **baking step**
  (sample at 400 K during 1h30 min before TDS and after the implantation)

- Quastel et al.: **Well defined experimental conditions** but high flux and fluence: **trap creation (different from vacancies)?**
Parameters used in the simulation

- fluence = $10^{21}$ D/m$^2$, flux = $10^{18}$ D/m$^2$/s, 500 eV/D, heating ramp = 5 K/s
- Resting time = 10 h and backing at 400 K during 1h30min just after the implantation (T of implantation = 300 K)

Detrapping energy used (DFT values):
- $E_1 = 1,406$ eV (1.43) (-2%)
- $E_2 = 1,402$ eV (1.42) (-1%)
- $E_3 = 1,202$ eV (1.25)
- $E_4 = 1,123$ eV (1.17)
- $E_5 = 1,065$ eV (1.10)
- $E_6 = 0.820$ eV (0.86)

$E_1$ and $E_2$ in agreement with DFT
Due to baking, no information at low temperature

N$_t$ = $5.5 \times 10^{-4}$
FIT OF EXPERIMENTAL DATA WITH MIHMS-RESERVOIR: THE QUASTEL’S DATA

Parameters used in the simulation

- fluence = 10^{23} \text{ D/m}^2, \text{ flux} = 10^{20} \text{ D/m}^2/\text{s}, 500 \text{ eV/D}, \text{ heating ramp} = 5,5 \text{ K/s}
- Resting time = 0,42 \text{ h} and no backing

The detrapping energy used (DFT values):
- \( E_1 = 1,31 \text{ eV} (1,43) (-8\%) \)
- \( E_2 = 1,30 \text{ eV} (1,42) (-8\%) \)
- \( E_3 = 1,19 \text{ eV} (1,25) (-5\%) \)
- \( E_4 = 1,17 \text{ eV} (1,17) (0\%) \)
- \( E_5 = 1,06 \text{ eV} (1,10) (-4\%) \)
- \( E_6 = 0,85 \text{ eV} (0,86) (-1\%) \)

- \( E_1 \) to \( E_6 \) in agreement with DFT and with previous test
THE MIMHS-RESERVOIR RESULTS

- MIHMS-reservoir able to fit TDS experimental data
- The detrapping energies obtained in agreement with DFT:

Need of new experiment on very well characterized SCW samples

Then, experiment with more complex crystal to discriminate between vacancies, Grain boundaries etc… : target of the WHISCI project
Comparison between OKMC (LAKIMOCA) and MHIMS-reservoirs, based on DFT results

Conditions:
- Sample of 300nm (1000W cells)
- Vacancies density: $2 \times 10^{-6}$
- At RT, vacancies filled by 6 H
- T ramp up: 1K/s

- TDS starts immediately (no resting time):
  - 3 peaks observed

- TDS starts after 1000s at 300K:
  - Disappearance of low temperature band
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• TDS starts immediately (no resting time):
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• TDS starts after 1000s at 300K:
  • Disappearance of low temperature band

Same results obtained with both codes (confidence on MHIMS-reservoir)
DFT predicts in SC:
- H trapping energy, H migration energy, total concentration of vacancies,…
CONCLUSIONS

- DFT predicts in SC:
  - H trapping energy, H migration energy, total concentration of vacancies,…

- MHIMS Macroscopic Rate Equation Model:
  - Large number of parameters 😞
  - Some ad hoc hypothesis on the traps density 😞 but ok for low flux 😊
  - However,
    - good data fitting 😊
    - Good crosschecked with other macroscopic codes 😊
    - Valuable extrapolation for laboratory studies 😊
      - tokamak studies (role of impurity in the ion flux and on the surface properties) 😞
CONCLUSIONS

- DFT predicts in SC:
  - H trapping energy, H migration energy, total concentration of vacancies,…

- MHIMS Macroscopic Rate Equation Model:

- MHIMS-reservoir Rate Equation Model:
  - Reduced number of parameters 😊
  - Strong links with basic physics (DFT) 😊
  - Good data fitting for SCW 😊 but small numbers of experiment 😞
  - Extrapolation to PCW? 😞 and to tokamak 😞

  ✓ The only way to proceed in order to address all the physical processes
CONCLUSIONS

- DFT predicts in SC:
  - H trapping energy, H migration energy, total concentration of vacancies,…

- MHIMS Macroscopic Rate Equation Model:

- MHIMS-reservoir Rate Equation Model:

- Comparison of OKMC/MRE modeling: excellent agreement 😊
CONCLUSIONS

- DFT predicts in SC:
  - H trapping energy, H migration energy, total concentration of vacancies,…

- MHIMS Macroscopic Rate Equation Model:

- MHIMS-reservoir Rate Equation Model:

- Comparison of OKMC/MRE modeling: excellent agreement 😊

- Future activities:
  - Improve data base of well characterized samples
    - On SCW and/or PCW
    - Well controlled surfaces + impurities effects
    - Well controlled implantation temperature and storage (down to 77K)
    - Neutrons simulation
    - Improving the MRE modeling
  - WEST application

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